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# THE TOPOLOGY AND GEOMETRY OF SELF-ADJOINT AND ELLIPTIC BOUNDARY CONDITIONS FOR DIRAC AND LAPLACE OPERATORS

M. Asorey

*Departamento de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza,  
 E-50009 Zaragoza, Spain.  
 asorey@unizar.es*

A. Ibort

*ICMAT & Depto. de Matemáticas, Universidad Carlos III de Madrid,  
 Avda. de la Universidad 30, E-28911 Leganés, Madrid, Spain.  
 albertoi@math.uc3m.es*

G. Marmo

*Dipartimento di Fisica, INFN Sezione di Napoli, Università di Napoli,  
 I-80125 Napoli, Italy.  
 marmo@na.infn.it*

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The theory of self-adjoint extensions of first and second order elliptic differential operators on manifolds with boundary is studied via its most representative instances: Dirac and Laplace operators.

The theory is developed by exploiting the geometrical structures attached to them and, by using an adapted Cayley transform on each case, the space  $\mathcal{M}$  of such extensions is shown to have a canonical group composition law structure.

The obtained results are compared with von Neumann's Theorem characterising the self-adjoint extensions of densely defined symmetric operators on Hilbert spaces. The 1D case is thoroughly investigated.

The geometry of the submanifold of elliptic self-adjoint extensions  $\mathcal{M}_{\text{ellip}}$  is studied and it is shown that it is a Lagrangian submanifold of the universal Grassmannian  $\mathbf{Gr}$ . The topology of  $\mathcal{M}_{\text{ellip}}$  is also explored and it is shown that there is a canonical cycle whose dual is the Maslov class of the manifold. Such cycle, called the Cayley surface, plays a relevant role in the study of the phenomena of topology change.

Self-adjoint extensions of Laplace operators are discussed in the path integral formalism, identifying a class of them for which both treatments leads to the same results.

A theory of dissipative quantum systems is proposed based on this theory and a unitarization theorem for such class of dissipative systems is proved.

The theory of self-adjoint extensions with symmetry of Dirac operators is also discussed and a reduction theorem for the self-adjoint elliptic Grassmannian is obtained.

Finally, an interpretation of spontaneous symmetry breaking is offered from the

2 *Contents*

point of view of the theory of self-adjoint extensions.

*Keywords:* Self-adjoint extensions, elliptic boundary conditions, Dirac operators, Laplace operators.

**Contents**

<b>1</b>	<b>Introduction</b>	<b>3</b>
<b>2</b>	<b>Self-adjoint extensions of first order elliptic operators: Dirac operators</b>	<b>8</b>
2.1	Dirac operators . . . . .	8
2.2	The geometric structure of the space of boundary data . . . . .	10
2.3	The Cayley transform on the boundary . . . . .	12
2.4	Simple examples: The Dirac operators in 1 and 2 dimensions . . . . .	14
<b>3</b>	<b>Self-adjoint extensions of Laplace operators</b>	<b>16</b>
3.1	The covariant Laplacian . . . . .	16
3.2	Complex structures on the Hilbert space of boundary data . . . . .	18
3.3	The Cayley transformation on the boundary Hilbert space for Laplacian operators . . . . .	20
3.4	Squaring the space of boundary conditions of Dirac operators and boundary conditions for Laplace operators . . . . .	23
<b>4</b>	<b>Von Neumann's theorem and boundary conditions revisited</b>	<b>27</b>
4.1	Von Neumann's theorem vs. unitary operators at the boundary . . . . .	27
4.2	Examples and applications: Boundary conditions for the Laplace operator in one-dimension . . . . .	31
4.2.1	Self-adjoint extensions of Schrödinger operators in 1D . . . . .	33
4.2.2	The spectral function . . . . .	34
4.2.3	Quantum wires and quantum Kirchhoff's law . . . . .	37
<b>5</b>	<b>Self-adjoint extensions and semiclassical boundary conditions</b>	<b>39</b>
5.1	Classical boundary conditions and path integrals . . . . .	39
5.2	Path integrals and quantum boundary conditions . . . . .	41
<b>6</b>	<b>The space of self-adjoint elliptic boundary conditions</b>	<b>44</b>
6.1	The elliptic Grassmannian . . . . .	44
6.2	The space of self-adjoint extensions: the self-adjoint Grassmannian and elliptic self-adjoint extensions . . . . .	47
<b>7</b>	<b>Self-adjoint extensions of dissipative systems</b>	<b>51</b>
7.1	Non-self-adjoint extensions and local evolution . . . . .	51
7.2	Unitarization of non-self-adjoint boundary conditions . . . . .	53

<b>8 Self-adjoint extensions of elliptic operators with symmetry</b>	<b>57</b>
8.1 Dirac bundles with symmetry . . . . .	57
8.2 The quotient Dirac operator . . . . .	58
8.3 Unitaries at the boundary and $G$ -invariance . . . . .	62
8.4 Examples: Groups acting by isometries . . . . .	63
8.5 Reduction of symplectic manifolds by fixed sets and the reduced elliptic Grassmannian . . . . .	67
8.6 The reduction of the Grassmannian and the space of virtual self- adjoint extensions . . . . .	70
<b>9 Spontaneous symmetry breaking and self-adjoint extensions</b>	<b>72</b>
9.1 The notion of spontaneous symmetry breaking . . . . .	72
9.2 The bifurcation diagram of the space of self-adjoint extensions . . .	74
<b>10 Conclusions and further developments</b>	<b>76</b>

## 1. Introduction

The construction and discussion of quantum mechanical systems requires a detailed analysis of the boundary conditions (BC) imposed on the system. Often such boundary conditions are imposed by the observers and their experimental setting or are inherent to the system. This is a common feature of all quantum systems, even the simpler ones.

The outcomes of measurable quantities of the system will change with the choice of BC because the spectrum of the quantum observables will vary with the different self-adjoint extensions obtained for them depending on the chosen BC.

The Correspondence Principle provides a useful guide to the analysis of quantum mechanical systems, but it is not obvious how it extends to include boundary conditions both in classical and quantum systems. For instance, Dirichlet's boundary conditions corresponds to impenetrability of the classical walls determining the boundary of the classical system in configuration space, but, what are the corresponding classical conditions for mixed BC? Then, we are facing the problem of determining the classical limit of quantum BC. Conversely, we can address the question of 'quantizing' classical boundary conditions. In particular we can ask if the classical determination of BC is enough to fully describe a 'quantized' system.

As the experimental and observational capabilities are getting more and more powerful, we are being forced to consider boundary conditions beyond the standard ones, Dirichlet, Neumann, etc. For instance, in Condensed matter, models with 'sticky' boundary conditions are seen to be useful to understand certain aspects in the Quantum Hall effect [Jo95]; in quantum gravity, self-adjoint extensions are used to understand signature change [Eg95]. Even more fundamental, topology change in quantum systems is modelled using dynamics on BC's [Ba95]. Physical implications of the problem were already analyzed in [As12].

Following Dirac's approach, we can develop a canonical quantization program

for classical systems with boundary. Such program requires a prior discussion on the dynamics of Hamiltonian systems with boundary.

Without entering a full discussion of this important problem, we may assume that a classical Hamiltonian system with boundary is specified by a Hamiltonian function  $H$  defined on the phase space  $T^*\Omega$  of a configuration space  $\Omega$  with boundary  $\partial\Omega$ , and a canonical transformation  $S$  of the symplectic boundary  $T^*\partial\Omega$ , obtained by considering the quotient of the restriction  $T^*_{\partial\Omega}\Omega$  of the cotangent bundle of  $\Omega$  to  $\partial\Omega$  and then, taking its quotient by the characteristic distribution of the restriction of the canonical symplectic structure on  $T^*\Omega$  to it. Thus, classical boundary conditions (CBC's) are defined by canonical maps

$$S: T^*\partial\Omega \rightarrow T^*\partial\Omega, \quad (1)$$

and form a group, the group of symplectic diffeomorphisms of  $T^*(\partial\Omega)^a$ .

Dirac's quantization rule will be stated as follows: Given a CBC  $S$ , and two classical observables  $f, g$  on  $T^*\Omega$ , determine a quantum boundary condition (QBC)  $\hat{S}$  and two self-adjoint operators  $\hat{f}_S, \hat{g}_S$  depending on  $\hat{S}$ , such that

$$[\hat{f}_S, \hat{g}_S] = i\hbar \widehat{\{f, g\}}_S, \quad (2)$$

and

$$\hat{S} \circ \hat{R} = \widehat{SR}, \quad (3)$$

where the composition on the left is a group composition on the space of QBC's to be discussed later on. It is obvious that as in the boundaryless situation such quantization rule could not be implemented for all observables and all CBC's. So, one important question for such program will be how to select subalgebras of classical observables and subgroups of CBC's suitable for quantization.

Before embarking in such enterprise, some relevant aspects of the classical and the quantum picture need to be clarified. For instance, we have to understand the structure of the self-adjoint extensions of the operator corresponding to a classical observable. The most important class of operators arising in the first quantization of classical systems are first and second order elliptic differential operators: the Laplace-Beltrami operator when quantizing a classical particle without spin, the Dirac operator for the quantization of particles with spin.

This family of operators are certainly the most fundamental of all elliptic operators, and in fact, in a sense all elliptic operators are obtained from them. Thus for Dirac and Laplace operators we will like to understand their self-adjoint realizations in terms of CBC's. For that we need to understand first their self-adjoint realizations in terms of QBC's.

Von Neumann developed a general theory of self-adjoint extensions of symmetric operators [Ne29]. Such theory is often presented in the realm of abstract Hilbert space theory that causes that the relevant features attached to the geometry of the

<sup>a</sup>Similar considerations can be made for more general classical phase space.

operators is lost. Thus we will proceed following a direct approach to the theory of self-adjoint extensions exploiting the geometry of first and second order elliptic differential operators, and obtaining a fresh interpretation of von Neumann's theory directly in terms of boundary data. A consequence of this analysis will be an interpretation of QBCs in terms of the unitary group at the boundary, that provides the group composition law needed for the implementation of Dirac's quantization rule Eq. (3).

Elliptic differential operators have been exhaustively studied culminating with the celebrated Atiyah-Singer index theorem that relates the analytical index of such operators with the topological invariants of the underlying spaces [At68]. Such analysis extends to the boundary situation provided that appropriate elliptic boundary conditions are used. A remarkable example is provided by the global elliptic boundary conditions introduced in [At75], or APS conditions, that allow to describe the index of Dirac operators on manifolds with boundary. Such extensions have been adequately generalized for higher order elliptic operators giving rise to interesting constructions of boundary data [Fr97]. We should also recall here the important contributions by Lesch and Wojciechowski on the theory of elliptic boundary conditions and spectral invariants and the geometry of the elliptic Grassmannian (see for instance [Le96]).

However, from a physical viewpoint another family of boundary conditions has been considered for quark fields in bag models of quark confinement in QCD. The theory of chiral boundary conditions is not well developed although many physical applications have been analyzed from this perspective [Ch74], [Rho83], [As13], [As15].

The program sketched so far concerns exclusively with first quantization of classical systems, but second quantization is needed to truly deal with their physical nature. First quantization of classical systems, requires to consider the quantization of boundary conditions, which leads automatically to consider a collection of QBC's for the first quantized system. Even for very simple systems, like a fermion propagating on a disk we need to consider 'all' self-adjoint extensions of Dirac's operator on the disk. Thus, to proceed to second quantization we need to understand the global structure of such space of extensions. We will show that such space lies naturally in the infinite dimensional Grassmannian manifold and defines a Lagrangian submanifold of it, that will be called the self-adjoint Grassmannian.

Such infinite dimensional Grassmannian was introduced in the study of the KdV and KP integrable hierarchies of nonlinear partial differential equations [Se85]. It represents a 'universal phase space' for a large class of integrable evolution problems. Lately, such infinite dimensional Grassmannian was introduced again as the phase space of string theory and its quantization was discussed [Al87], [Wi88].

Our approach here is different, the infinite dimensional Grassmannian appears as the natural setting to discuss simultaneously all QBC's for a first quantized classical system of arbitrary dimension. In fact, the relevant QBC's are contained in a Lagrangian submanifold of the elliptic Grassmannian that should be subjected

to second quantization. Lagrangian submanifolds of symplectic manifolds play the role of ‘generalized functions’, thus such program would imply quantizing a particular observable of the Grassmannian, making contact again with string theory. We should stress here that string theory is genuinely 2D whereas we are dealing with a classical point-like theory for classical objects in arbitrary dimensions.

The realization of such program would eventually introduce quantum dynamical effects on the space of QBC’s, suggesting that QBC’s could actually change (as suggested in [Ba95]), or that there is the possibility of non-vanishing probability amplitudes between states characterized by different boundary conditions. This observation imply that probably our first statement concerning the structure of classical systems with boundary is not totally correct, and we should extend it as follows: In the boundaryless situation, a Hamiltonian function defines a flow of symplectic diffeomorphisms  $\phi_t$  on the phase space of the system. We must replace then the specification of CBC’s by a fixed symplectic diffeomorphism on the boundary and to allow for a flow of symplectic diffeomorphisms on the boundary too, i.e., by a boundary Hamiltonian  $H_B$ . Upon quantization such Hamiltonian will define a quantum Hamiltonian on the space of QBC’s that eventually will lead to a propagator on second quantization.

Apart from the difficulties and physical implications of such ideas, we must point out an immediate consequence related to the topology of the systems studied. Changing the classical and quantum boundary conditions implies that possibility of changes in the topology of the system. For instance the quantization of a fermion moving on a disk with changing boundary conditions can change the topology of the disk and evolve into a surface of higher genus. Such process was analyzed by Asorey, Ibort and Marmo [As05] and it was shown that in the first quantized scheme such change can only occur if the trajectory in the space of self-adjoint extensions of the system cuts a submanifold where the spectrum of the operator diverges. Such submanifold is called the Cayley submanifold and describes its topology. Thus, in this sense the Cayley submanifold acts as a ‘wall’ in the space of QBC’s for a first quantized system with boundary, even though this will not preclude tunnelling in second quantization (see also [Sh12] for arguments along similar lines).

There are many other physical phenomena involving the ‘boundary’ of physical systems that it would be simply impossible to enumerate here. We would just like to mention a few recent contributions related to different physical problems: the analysis of boundary conditions and the Casimir effect in [As06], [As07], the role of boundary conditions in topological insulators [As13], and boundary conditions generated entanglement [Ib14b].

In this work we will try to offer a panorama of the field by presenting a discussion on some fundamental aspects of the theory of self-adjoint extensions of Laplace and Dirac-like operators, as well as a variety of related ideas and problems still on development. There is a vast literature on the subject covering its mathematical flank and it would be impossible to reproduce here. We must cite however, apart from the reference to the work by von Neumann already quoted, the pioneering

work by Weyl [We09], Friedrichs' construction [Fr34] or the contributions by Krein and Naimark [Kr47, Na43] to the general theory as a few historical landmarks.

On the other hand the theory of extensions of elliptic operators has attracted a lot of attention and, apart from the index theorem related works cited above, there is a number of fundamental results on the fields. We will just quote the analysis of non-local extensions of elliptic operators by Grubb [Gr68] and the theory of singular perturbations of differential operators by Albeverio and Kurasov [Al99] because of their influence on this work (see also [Ib14] for a quadratic forms based analysis of the extensions of the Laplace-Beltrami operator and [Ib12] where the reader will find a reasonable list of references on the subject).

Thus, we will proceed by reviewing first the geometric theory of self-adjoint extensions of Dirac and Laplace operators where the role of the Cayley transform at the boundary will be emphasized and the group structure of the space of self-adjoint extensions will be described explicitly. This will be the content of Sects. 2 and 3. Afterwards, Section 4 the relation with von Neumann's theorem will be discussed and the one-dimensional situation will be discussed thoroughly. The spectral function for arbitrary boundary conditions will be obtained explicitly and the quantum analogue of Kirchhoff's laws will be obtained.

In Section 5 we will begin to discuss the semiclassical theory of self-adjoint extensions and its implementation in the path integral representation of quantum systems. Section 6 will be devoted to study the global structure of the space of extensions both elliptic and self-adjoint. The infinite-dimensional Grassmannian will be discussed as well as the Lagrangian submanifold of elliptic self-adjoint extensions.

We will introduce the study of dissipative quantum systems via non-self-adjoint boundary conditions in Section 7 where a unitarization theorem for dissipative systems will be stated.

The problem of dealing with symmetries of quantum systems will be addressed in Section 8, that is, if the quantum system has a symmetry, which are the self-adjoint extensions compatible with it. This problem will be stated and partially solved (see also [Ib14c]) and some examples will be exhibited. Particular attention will be paid to the space of self-adjoint extensions of the quotient Dirac operator of a Dirac operator with symmetry and its characterization as the symplectic manifold of fixed points of the self-adjoint Grassmannian.

It could also happen that even if we have a symmetry of a symmetric operator, the self-adjoint extension describing the corresponding quantum system will not share the same symmetry. We will say then that there is a spontaneous breaking of the symmetry. This situation will be succinctly dealt with in Section 9.

## 2. Self-adjoint extensions of first order elliptic operators: Dirac operators

### 2.1. Dirac operators

As it was indicated before, Dirac operators constitute an important class of first order elliptic operators, to the extent that most relevant elliptic operators arising in geometry and physics are directly related to them. Let us set the ground for them. We will consider a Riemannian manifold  $(\Omega, \eta)$  with smooth boundary  $\partial\Omega$ . We denote by  $\text{Cl}(\Omega)$  the Clifford bundle over  $\Omega$ , defined as the algebra bundle whose fibre at  $x \in \Omega$  is the Clifford algebra  $\text{Cl}(T_x\Omega)$  generated by vectors  $u$  in  $T_x\Omega$  with relations

$$u \cdot v + v \cdot u = -2\eta(u, v)_x, \quad \forall u, v \in T_x\Omega.$$

Let  $\pi: S \rightarrow \Omega$  be a  $\text{Cl}(\Omega)$ -complex vector bundle over  $\Omega$ , i.e., for each  $x \in \Omega$ , the fibre  $S_x = \pi^{-1}(x)$  is a  $\text{Cl}(\Omega)_x$ -module, or in other words, there is a representation of the algebra  $\text{Cl}(\Omega)_x = \text{Cl}(T_x\Omega)$  on the complex space  $S_x$ . We will indicate by  $u \cdot \xi$  the action of the element  $u \in \text{Cl}(\Omega)_x$  on the vector  $\xi \in S_x$ . We will also assume in addition that the bundle  $S$  carries a hermitian metric denoted by  $(\cdot, \cdot)$  such that Clifford multiplication by unit vectors in  $T\Omega$  is unitary, that is,

$$(u \cdot \xi, u \cdot \zeta)_x = (\xi, \zeta)_x, \quad \forall \xi, \zeta \in S_x, u \in T_x\Omega, \|u\|^2 = 1. \quad (4)$$

Finally, we will assume that there is a Hermitean connection  $\nabla$  on  $S$  such that

$$\nabla(V \cdot \xi) = (\nabla_\eta V) \cdot \xi + V \cdot \nabla \xi, \quad (5)$$

where  $V$  is a smooth section of the Clifford bundle  $\text{Cl}(\Omega)$ ,  $\xi \in \Gamma(S)$  and  $\nabla_\eta$  denotes the canonical connection on  $\text{Cl}(\Omega)$  induced by the Riemannian structure  $\eta$  on  $\Omega$ .

A bundle  $\pi: S \rightarrow \Omega$  with the structure described above is commonly called a Dirac bundle [La89] and they provide the natural framework to define Dirac operators. Thus, if  $\pi: S \rightarrow \Omega$  is a Dirac bundle, we can define a canonical first-order differential operator  $\not{D}: \Gamma(S) \rightarrow \Gamma(S)$  by setting:

$$\not{D}\xi = e_j \cdot \nabla_{e_j} \xi, \quad (6)$$

where  $e_j$  is any orthonormal frame at  $x \in \Omega$ .

There is a natural inner product on the space of smooth sections  $\Gamma(S)$  of the Dirac bundle  $S$  induced from the pointwise inner product  $(\cdot, \cdot)$  on  $S$  by setting

$$\langle \xi, \zeta \rangle = \int_{\Omega} (\xi(x), \zeta(x))_x \text{vol}_\eta(x),$$

where  $\text{vol}_\eta$  is the volume form defined by the Riemannian structure on  $\Omega$ . We will denote the associated norm by  $\|\cdot\|_2$  and  $L^2(\Omega, S)$  is the corresponding Hilbert space of square integrable sections of  $S$ .

The Dirac operator  $\not{D}$  is defined on the Frechet space of smooth sections of  $S$ ,  $\Gamma(S)$ , however this is not the largest domain where it can be defined. The largest



domain in  $L^2(\Omega, S)$  where this operator can be defined consists of the completion of  $\Gamma(S)$  with respect to the Sobolev norm  $\|\cdot\|_{1,2}$  defined by

$$\|\xi\|_{k,2}^2 = \int_{\Omega} (\xi(x), (I + \nabla^\dagger \nabla)^{k/2} \xi(x))_x \text{vol}_\eta(x), \quad (7)$$

with  $k = 1$ , where  $\nabla^\dagger$  is the adjoint operator to  $\nabla$  in  $L^2(\Omega, S)$ . In fact, such space is the space of sections of  $S$  possessing first weak derivatives which are in  $L^2(\Omega, S)$ . This Hilbert space will be denoted by  $H^1(\Omega, S)$  (see for instance [Ad03]).

The operator  $\mathcal{D}$  defined on  $H^1(\Omega, S)$  is not self-adjoint as we will discuss in what follows. However it is immediate to check that the Dirac operator is symmetric in  $\Gamma_0(\overset{\circ}{S})$ , the space of smooth sections of  $S$  with compact support contained in  $\overset{\circ}{\Omega}$ , the interior of  $\Omega$ . In fact, after an integration by parts we obtain immediately,

$$\langle \mathcal{D}\sigma, \rho \rangle = \langle \sigma, \mathcal{D}\rho \rangle, \quad \forall \sigma, \rho \in \Gamma_0(\overset{\circ}{S}). \quad (8)$$

The operator  $\mathcal{D}$  with this domain is closable on  $H^1(\Omega, S)$  and its closure is the completion of  $\Gamma_0(\overset{\circ}{S})$  with respect to the norm  $\|\cdot\|_{1,2}$ . Such domain will be denoted by  $H_0^1(\Omega, S) \subset H^1(\Omega, S)$ . The elements of  $H_0^1(\Omega, S)$  are sections vanishing on  $\partial\Omega$  with  $L^2$ -weak derivatives. Notice that both  $H_0^1(\Omega, S)$  and  $H^1(\Omega, S)$  are dense subspaces in  $L^2(\Omega, S)$ .

If we denote by  $\mathcal{D}_0$  the closure of  $\mathcal{D}$  on  $H_0^1(S)$ , it is simple to check that  $\mathcal{D}_0^\dagger = \mathcal{D}$  with domain  $H^1(\Omega, S)$ , where  $\mathcal{D}_0^\dagger$  denotes the adjoint of  $\mathcal{D}_0$  in  $L^2(S)$ . The domains of the different self-adjoint extensions, if any, of  $\mathcal{D}_0$  will be linear dense subspaces of  $H^1(\Omega, S)$  containing  $H_0^1(\Omega, S)$  such that the boundary terms obtained in the integration by parts procedure will vanish. We will denote in what follows by  $\text{Dom}(T)$  the domain of the operator  $T$  and by  $\text{Ran}(T)$  its range, then the symmetric extensions  $\mathcal{D}_s$  of  $\mathcal{D}_0$  will be defined on subspaces  $\text{Dom}(\mathcal{D}_s)$  such that

$$H_0^1(\Omega, S) = \text{Dom}(\mathcal{D}_0) \subset \text{Dom}(\mathcal{D}_s) \subset \text{Dom}(\mathcal{D}_s^\dagger) \subset \text{Dom}(\mathcal{D}) = H^1(\Omega, S),$$

and  $\mathcal{D}_s \xi = \mathcal{D} \xi$  for any  $\xi \in \text{Dom}(\mathcal{D}_s)$ . A self-adjoint extension of  $\mathcal{D}$  is a symmetric extension  $\mathcal{D}_s$  of  $\mathcal{D}_0$  such that  $\text{Dom}(\mathcal{D}_s) = \text{Dom}(\mathcal{D}_s^\dagger)$ .

We will characterize such self-adjoint extensions by using first the geometry of some Hilbert spaces defined on the boundary of  $\Omega$  and, later on, we will compare with the classical theory of self-adjoint extensions of densely defined symmetric operators developed by von Neumann [Ne29]. To do that, we will repeat first the well-known integration by part process used to derive formula (8).

Let  $x \in \Omega$  and  $\{e_j\}$  an orthonormal frame in a neighborhood of  $x$  so that  $\nabla_{e_j} e_i = 0$  at  $x$  for all  $i, j$ . If  $\xi, \zeta$  are sections of  $S$ , then they define a vector field  $X$  in a neighborhood of  $x$  by the condition

$$\eta(X, Y) = -(\xi, Y \cdot \zeta), \quad \forall Y.$$

Then, at  $x$ , we get:

$$\langle \mathcal{D}\xi, \zeta \rangle = \langle e_j \nabla_{e_j} \xi, \zeta \rangle = -\nabla_{e_j} \langle \xi, e_j \zeta \rangle + \langle \xi, \mathcal{D}\zeta \rangle,$$

10 *M. Asorey, A. Ibor, G. Marmo*

but, by definition  $\operatorname{div}(X) = \eta(\nabla_{e_j} X, e_j)$ , hence,

$$\operatorname{div}(X) = \nabla_{e_j} \eta(X, e_j) - \eta(X, \nabla_{e_j} e_j) = -(e_j \cdot \xi, e_j \cdot \zeta).$$

Namely,

$$(\not{D}\xi(x), \zeta(x))_x - (\xi(x), \not{D}\zeta(x))_x = \operatorname{div}_x(X).$$

Integrating both parts of the equation, we will find,

$$\langle \not{D}\xi, \zeta \rangle - \langle \xi, \not{D}\zeta \rangle = \int_{\Omega} \operatorname{div}_x(X) \operatorname{vol}_{\eta}(x) = \int_{\Omega} d(i_X \operatorname{vol}_{\eta}) = \int_{\partial\Omega} i^*(i_X \operatorname{vol}_{\eta}),$$

where we denote by  $i: \partial\Omega \rightarrow \Omega$  the canonical inclusion. If  $\nu$  denotes the inward unit vector on the normal bundle to  $\partial\Omega$ , the volume form  $\operatorname{vol}_{\eta}$  can be written as  $\theta \wedge \operatorname{vol}_{\partial\Omega}$ , where  $\operatorname{vol}_{\partial\Omega}$  is an extension of the volume form defined on  $\partial\Omega$  by the restriction of the Riemannian metric  $\eta$  to it, and  $\theta$  is a 1-form such that  $\theta(Y) = \eta(Y, \nu)$ . Then we easily get,

$$i_X \operatorname{vol}_{\eta} = (i_X \theta) \operatorname{vol}_{\partial\Omega} = \eta(X, \nu) \operatorname{vol}_{\partial\Omega} = (\xi, \nu \cdot \zeta) \operatorname{vol}_{\partial\Omega},$$

and, finally, we get

$$\langle \not{D}\xi, \zeta \rangle - \langle \xi, \not{D}\zeta \rangle = \int_{\partial\Omega} i^*(\nu \cdot \xi, \zeta) \operatorname{vol}_{\partial\Omega}. \quad (9)$$

## 2.2. The geometric structure of the space of boundary data

We will denote by  $S_{\partial\Omega}$  the restriction of the Dirac bundle  $S$  to  $\partial\Omega$ , i.e.,  $\pi_{\partial\Omega}: S_{\partial\Omega} = S|_{\partial\Omega} = i^*S \rightarrow \partial\Omega$ ,  $\pi_{\partial\Omega}(\xi) = \pi(\xi)$  for any  $\xi \in S_x$ ,  $x \in \partial\Omega$ . Notice that  $S_{\partial\Omega}$  becomes a Dirac bundle over  $\partial\Omega$ . It inherits an inner product  $(\cdot, \cdot)$  induced from the Hermitean product on  $S$  as well as an Hermitean connection  $\nabla_{\partial\Omega}$ , defined again by restricting the connection  $\nabla$  on  $S$  to sections along  $\partial\Omega$ . Thus the boundary Dirac bundle  $S_{\partial\Omega}$ , carries a canonical Dirac operator denoted by  $\not{D}_{\partial\Omega}$ .

Notice that  $\partial\Omega$  is a manifold without boundary, thus the boundary Dirac operator is essentially self-adjoint and has a unique self-adjoint extension (see [La89], Thm. 5.7). We shall use this fact later on.

We will denote as before by  $L^2(\partial\Omega, S_{\partial\Omega})$  the Hilbert space of square integrable sections of  $S_{\partial\Omega}$  and by  $\langle \cdot, \cdot \rangle_{\partial\Omega}$  its Hilbert product structure:

$$\langle \phi, \psi \rangle_{\partial\Omega} = \int_{\partial\Omega} (\phi(x), \psi(x))_x \operatorname{vol}_{\partial\Omega}(x), \quad \psi, \phi \in L^2(\partial\Omega, S_{\partial\Omega}). \quad (10)$$

Because of Lions trace theorem [Li72] the restriction map  $i^*: \Gamma(S) \rightarrow \Gamma(S_{\partial\Omega})$ ,  $\sigma \mapsto \phi = i^*\sigma$ , extends to a continuous linear map:

$$b: H^1(\Omega, S) \rightarrow H^{1/2}(\partial\Omega, S_{\partial\Omega}).$$

The Hilbert space  $H^{1/2}(\partial\Omega, S_{\partial\Omega})$  will be called the Hilbert space of boundary data for the Dirac operator  $\not{D}$  and will be denoted in what follows by  $\mathcal{H}_D$ . It carries an interesting extra geometrical structure induced by the boundary form defined by

Green's formula (9) responsible for the non self-adjointness of the Dirac operator  $\not{D}$  in  $H^1(\Omega, S)$ .

$$\Sigma(\phi, \psi) = \int_{\partial\Omega} (\nu(x) \cdot \phi(x), \psi(x))_x \text{vol}_{\partial\Omega}(x). \quad (11)$$

The normal vector field  $\nu$  defines an automorphism of the Dirac bundle  $S_{\partial\Omega}$  and an isomorphism:

$$\nu: \Gamma(S_{\partial\Omega}) \rightarrow \Gamma(S_{\partial\Omega}),$$

by  $\nu(\phi)(x) = \nu(x) \cdot \phi(x)$ , for all  $x \in \partial\Omega$ ,  $\phi \in \Gamma(S_{\partial\Omega})$ . Such automorphism extends to a continuous complex linear operator of  $\mathcal{H}_D$  denoted now by  $J$ . Because  $\nu^2 = -1$  in the Clifford algebra, such operator  $J$  verifies  $J^2 = -I$ . In addition, because of the Dirac bundle structure, eq. (4),  $J$  is an isometry of the Hilbert space product,

$$\langle J\phi, J\psi \rangle_{\partial\Omega} = \langle \phi, \psi \rangle_{\partial\Omega}, \quad \forall \phi, \psi \in \mathcal{H}_D, \quad (12)$$

i.e.,  $J$  defines a compatible complex structure on  $\mathcal{H}_D$ . In general, a complex Hilbert space  $\mathcal{H}$  with inner product  $\langle \cdot, \cdot \rangle$  and a compatible complex structure  $J$  defines a new continuous bilinear form  $\omega$  by setting,

$$\omega(\varphi, \psi) = \langle J\varphi, \psi \rangle, \quad \forall \varphi, \psi \in \mathcal{H}.$$

Such structure is skew-hermitian in the sense that

$$\omega(\varphi, \psi) = -\overline{\omega(\psi, \varphi)}.$$

(Notice that in the real case  $\omega$  will define a symplectic structure on  $\mathcal{H}$ .) We will call such structure  $\omega$  symplectic-Hermitean and the corresponding linear space a symplectic hermitian linear space (see for instance [Ha00] for a discussion of finite-dimensional Hermitian symplectic geometry).

The compatible complex structure allows to decompose the Hilbert space  $\mathcal{H}$  as

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-, \quad (13)$$

where  $\mathcal{H}_{\pm}$  are the  $\mp i$  eigenspaces of  $J$ , that is  $\phi_{\pm} \in \mathcal{H}_{\pm}$  if  $J\phi_{\pm} = \mp i\phi_{\pm}$ . The subspaces  $\mathcal{H}_{\pm}$  are orthogonal as the following computation shows.

$$\langle \phi_+, \phi_- \rangle = \langle J\phi_+, J\phi_- \rangle = \langle i\phi_+, -i\phi_- \rangle = -\langle \phi_+, \phi_- \rangle$$

The Hilbert space  $\mathcal{H}$  will carry in this way a natural decomposition in two orthogonal infinite dimensional closed subspaces, i.e., a polarization. Notice that the Hilbert space  $\mathcal{H}_D$  carries already another complex structure, denoted by  $J_0$ , multiplication by  $i$ , and both complex structures are also compatible in the sense that  $[J, J_0] = 0$ . because of the bundle  $S$  is a  $\text{Cl}(\Omega)$  complex bundle. In addition this implies that

$$J(\mathcal{H}_+ \pm i\mathcal{H}_-) \subset \mathcal{H}_{\pm}.$$

Hence, the Hilbert space of boundary data  $\mathcal{H}_D$  for the Dirac operator  $\mathcal{D}$  is a polarized Hilbert space carrying a compatible complex structure  $J_D$  and the corresponding symplectic-hermitian structure  $\omega_D$ . Using these structures the boundary form  $\Sigma$  is written as,

$$\Sigma(\xi, \zeta) = \omega(b(\xi), b(\zeta)) = \langle Jb(\xi), b(\zeta) \rangle_{\partial\Omega}, \quad \forall \xi, \zeta \in \mathcal{H}^1(S). \quad (14)$$

From this characterization we immediately see that self-adjoint extensions  $\mathcal{D}_s$  of  $\mathcal{D}$  will be obtained in domains  $\text{Dom}(\mathcal{D}_s)$  such that their boundary image,  $b(\text{Dom}(\mathcal{D}_s))$  will be isotropic subspaces of  $\omega_D$ , thus vanishing the r.h.s. of Eq. (14). Moreover to be self-adjoint, such domains must verify that  $b(\text{Dom}(\mathcal{D}_s)) = b(\text{Dom}(\mathcal{D}_s^\dagger))$ , thus, they must be maximal subspaces with this property. We have thus proved the first part of the following theorem,

**Theorem 1.** *Self-adjoint extensions of the Dirac operator  $\mathcal{D}$  are in one to one correspondence with maximally closed  $\omega_D$ -isotropic subspaces of the boundary Hilbert space  $\mathcal{H}_D$ . The domain of any of these extensions is the inverse image by the boundary map  $b$  of the corresponding isotropic subspace. Moreover, each maximally closed  $\omega_D$ -isotropic subspace  $W$  of  $\mathcal{H}_D$  defines an isometry  $U: \mathcal{H}_+ \rightarrow \mathcal{H}_-$ , called the Cayley transform of  $W$  and conversely.*

**Proof.** Let  $W$  be a closed  $\omega_D$ -isotropic subspace of  $\mathcal{H}_D$ . Then,  $b^{-1}(W)$  is a closed subspace of  $H^1(\Omega, S)$  containing  $H_0^1(\Omega, S)$ . Let  $\mathcal{D}_W$  be the extension of  $\mathcal{D}$  defined on  $b^{-1}(W)$  and compute  $\mathcal{D}_W^\dagger$ . If  $b(\xi), b(\zeta) \in W$ , then  $\langle \mathcal{D}_W^\dagger \xi, \zeta \rangle = \langle \xi, \mathcal{D}_W \zeta \rangle + \omega(b(\xi), b(\zeta)) = \langle \xi, \mathcal{D}_W \zeta \rangle$  because  $W$  is  $\omega_D$  isotropic. This shows that  $b^{-1}(W) \subset \text{Dom}(\mathcal{D}_W^\dagger)$ . If there were  $\xi \in \text{Dom}(\mathcal{D}_W^\dagger) - b^{-1}(W)$ , then, the same computation shows that  $\omega_D(b(\xi), \phi) = 0$  for all  $\phi \in W$ , and the subspace  $W' = W \oplus \langle b(\xi) \rangle$  will be  $\omega_D$ -isotropic, which is contradictory. Thus  $\text{Dom}(\mathcal{D}_W) = \text{Dom}(\mathcal{D}_W^\dagger)$  and the extension is self-adjoint. The converse is proved similarly.

Let us consider now a closed maximal  $\omega_D$ -isotropic subspace  $W$ . Let us show that  $W$  is transverse to  $\mathcal{H}_\pm$ . Let  $\phi \in W \cap \mathcal{H}_\pm$ , then  $0 = \omega_D(\phi, \phi) = \langle J\phi, \phi \rangle = \mp i \|\phi\|^2$ , then  $\phi = 0$ . Then, the subspace  $W$  defines the graph of a continuous linear operator  $U: \mathcal{H}_+ \rightarrow \mathcal{H}_-$  and vectors  $\phi = \phi_+ + \phi_- \in W$  have the form  $\phi_- = U\phi_+$ . Then, the  $\omega_D$ -isotropy of  $W$  implies,

$$\begin{aligned} 0 &= \omega_D(\phi_+ + U\phi_+, \psi_+ + U\psi_+) \\ &= \langle i\phi_+ - iU\phi_+, \psi_+ + U\psi_+ \rangle = -i\langle \phi_+, \psi_+ \rangle + i\langle U\phi_+, U\psi_+ \rangle, \end{aligned}$$

for every  $\phi_+, \psi_- \in \mathcal{H}_+$ , that proves that  $U$  is unitary.  $\square$

### 2.3. The Cayley transform on the boundary

Theorem 1 is the boundary analogue of Von Neumann's description of selfadjoint extensions by means of isometries between the deficiency spaces  $\mathcal{N}_\pm$  (see later on). In spite of the inherent interest of this result, it is well-known that sometimes it

is more useful to have an alternative description of such extensions in terms of selfadjoint operators. For that we will use the Cayley transform. We shall define the Cayley transform on the polarized boundary Hilbert space  $\mathcal{H}_D = \mathcal{H}_+ \oplus \mathcal{H}_-$  as the isomorphism  $C: \mathcal{H}_D \rightarrow \mathcal{H}_D$  defined by  $C(\phi_1, \phi_2) = (\phi_1 + i\phi_2, \phi_1 - i\phi_2)$ , for every  $\phi_1 \in \mathcal{H}_+$ ,  $\phi_2 \in \mathcal{H}_-$ . The complex structure  $J_D$  is transformed into  $C^{-1}J_DC(\phi_1, \phi_2) = (-\phi_2, \phi_1)$  and the symplectic-hermitian structure  $\omega_D$  is transformed into the bilinear form

$$\sigma_D(\phi_1, \phi_2; \psi_2, \psi_2) = 2i(\langle \phi_2, \psi_2 \rangle - \langle \phi_1, \psi_2 \rangle). \quad (15)$$

Let  $U$  be a unitary operator  $U: \mathcal{H}_+ \rightarrow \mathcal{H}_-$  such that  $I - U$  is invertible. Then we have  $\phi_- = U\phi_+$  and using the Cayley transform,  $\phi_{\pm} = \phi_1 \pm i\phi_2$ , we will obtain that,

$$\phi_1 = i \frac{I + U}{I - U} \phi_2,$$

that defines an operator  $A_U: \mathcal{H}_+ \rightarrow \mathcal{H}_-$ . In general it will be more convenient to consider graphs of operators  $\mathcal{H}_+ \rightarrow \mathcal{H}_-$  because  $C$  acts on  $\mathcal{H}_D$ , then it actually maps subspaces of  $\mathcal{H}_D$  in subspaces of  $\mathcal{H}_D$ .

If  $W$  is a subspace of  $\mathcal{H}_D$ , then the adjoint of  $W$  will be the subspace  $W^\dagger$  defined by setting,

$$W^\dagger = \{ (\psi_1, \psi_2) \in \mathcal{H}_+ \oplus \mathcal{H}_- \mid \langle \phi_1, \psi_2 \rangle = \langle \phi_2, \psi_1 \rangle, \quad \forall (\phi_1, \phi_2) \in \mathcal{H}_+ \oplus \mathcal{H}_- \}.$$

The subspace  $W$  is said to be symmetric if  $W \subset W^\dagger$  and self-adjoint if  $W = W^\dagger$ . (see [Ar61] for more details on operational calculus with closed subspaces of a Hilbert space). We will say that an operator  $A: \mathcal{H}_+ \rightarrow \mathcal{H}_-$  is selfadjoint if its graph is a selfadjoint subspace of  $\mathcal{H}_D$ . In this sense it is obvious that the Cayley transform operator  $A_U$  of  $U$  is selfadjoint. Moreover, it is clear that self-adjoint subspaces are maximally isotropic subspaces of the bilinear form  $\sigma_D$  given by Eq. (15). But  $\sigma_D$  is the transformed bilinear form on  $\mathcal{H}_D$  by the Cayley transform, then, maximally  $\sigma_D$ -isotropic subspaces correspond to maximally  $\omega_D$ -isotropic subspaces, that is the Cayley transform maps one-to-one graphs of isometries  $U: \mathcal{H}_+ \rightarrow \mathcal{H}_-$  into self-adjoint subspaces of  $\mathcal{H}_D$ .

Let us denote by  $K: \mathcal{H}_+ \rightarrow \mathcal{H}_-$  a compact operator, we denote by  $W + K$  the subspace of  $\mathcal{H}_D$  given by  $\{ (\phi, \psi + K(\phi)) \mid (\phi, \psi) \in W \}$  and we will call it a compact deformation of  $W$ . If we denote by  $\mathcal{M}_D$  the space of self-adjoint subspaces of  $\mathcal{H}_D = \mathcal{H}_+ \oplus \mathcal{H}_-$ . We will introduce a topology in  $\mathcal{M}_D$  as follows. We shall define base for the topology by the family of balls given by the sets of subspaces of the form  $\mathcal{O}_{W, \epsilon} = \{ W + K \mid \|K\| < \epsilon, (W + K)^\dagger = W + K \}$ . Hence  $\mathcal{M}_D$  becomes a topological space (in fact as we will see later a smooth manifold).

We can summarize the previous discussion in the following theorem.

**Theorem 2.** *The Cayley transform defines a homeomorphism between the space of isometries  $U(\mathcal{H}_+, \mathcal{H}_-)$  from  $\mathcal{H}_+$  to  $\mathcal{H}_-$  with the operator topology and the space of self-adjoint subspaces of  $\mathcal{H}_D = \mathcal{H}_+ \oplus \mathcal{H}_-$ . Moreover, the self-adjoint extensions*

of the Dirac operator  $\not{D}$  are in one-to-one correspondence with the self-adjoint subspaces in  $\mathcal{M}_D$ .

#### 2.4. Simple examples: The Dirac operators in 1 and 2 dimensions

Consider  $\Omega$  a 1-dimensional manifold with boundary, hence a connected component may be either the half-line or a closed interval in the compact case. We may assume without loss of generality that the metric is constant. Then the Clifford bundle becomes the trivial bundle complex line bundle over  $\Omega$ , as  $\text{Cl}(1)$  is algebra isomorphic to  $\mathbb{C}$ . Hence Dirac's operator is simply  $\not{D} = i\partial/\partial x$ , i.e., the momentum operator.

Notice that if  $\Omega$  is the half-line  $[0, +\infty)$ , there are no self-adjoint extensions of  $D$ . The Hilbert space of boundary data is simply  $\mathcal{H}_D = \mathbb{C}$ . Then, Eq. (9) becomes:

$$\langle \not{D}\xi, \zeta \rangle - \langle \xi, \not{D}\zeta \rangle = -i\bar{\xi}(0)\zeta(0),$$

but, the only symmetric extensions are given by the condition  $\xi(0) = 0$ , i.e., functions in  $H_0^1(\Omega)$ , but such domain defines just a symmetric operator in full agreement with von Neuman's theorem (see later Sect. 4).

However, if  $\Omega$  is a closed interval  $[a, b]$ , then  $\mathcal{H}_D \cong \mathbb{C}^2$  and

$$\langle \not{D}\xi, \zeta \rangle - \langle \xi, \not{D}\zeta \rangle = i(\bar{\xi}(b)\zeta(b) - \bar{\xi}(a)\zeta(a)).$$

Notice that  $\mathcal{H}_{\pm} \cong \mathbb{C}$  and the space of self-adjoint extensions is given by unitary maps from  $\mathcal{H}_+$  to  $\mathcal{H}_-$ , that is  $U(1)$  (see also Sections 3.4 and 4.2 for a discussion on the relation between the self-adjoint extensions of  $\not{D}$  and the Laplace operator  $\Delta$ )

Dirac operators in 2D have been the subject of exhaustive research both from the mathematical and physical side. We will consider  $\Omega$  to be now a two dimensional compact orientable manifold, i.e., a Riemann surface  $\Sigma$  with boundary  $\partial\Sigma = \cup_{\alpha=1}^r S_{\alpha}$  where  $S_{\alpha} \cong S^1$ . Consider now a Dirac bundle  $S \rightarrow \Sigma$ . Notice that because of the general previous considerations  $S$  carries a representation of the Clifford algebra bundle  $\text{Cl}(\Sigma)$ .

Take a point  $p \in \Sigma$  and a local chart  $(U, p)$  around it with local complex coordinates  $z = x + iy$ . The tangent space  $T_p\Sigma$  is spanned by the local vector fields  $e_1 = \partial/\partial x$ ,  $e_2 = \partial/\partial y$ , and the two vectors can be taken to be orthonormal. Hence the Clifford algebra at  $p$  is generated by  $e_1, e_2$  with the relation:

$$e_1 \cdot e_2 + e_2 \cdot e_1 = 0, \quad e_1^2 = -1, \quad e_2^2 = -1.$$

The generators  $e_1, e_2$  of the Clifford algebra act on the tangent bundle as the  $2 \times 2$  matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}.$$

This representation happens to be the spinor representation of the spin group  $\text{Spin}(1)$  which is a double covering of  $U(1)$  (the covering  $U(1) \rightarrow U(1)$  given by

the map  $z \mapsto z^2$ ). Thus if we take the complexified tangent space  $T\Sigma \otimes \mathbb{C}$  as a Dirac bundle then we will have for the Dirac operator:

$$\not{D} = e_1 \cdot \nabla_{e_1} + e_2 \cdot \nabla_{e_2} = \begin{pmatrix} 0 & \bar{\partial} + A \\ \partial + \bar{A} & 0 \end{pmatrix},$$

with  $\partial, \bar{\partial}$  being the Cauchy–Riemann operators on the variables  $x, y$ , and  $A$  the homogeneous part of the Levi–Civita connection corresponding to the given Riemannian metric on  $\Sigma$ .

The  $\text{Cl}(2)$  representation above is reducible because  $\Gamma_5 = ie_1e_2$  anticommutes with  $e_1$  and  $e_2$ . In fact,  $\Gamma_5 = \sigma_3$  which has eigenvalues  $\pm 1$ . The representation space of  $\text{Cl}(2)$  decomposes into two subspaces  $S^\pm$  of eigenvectors of  $\pm 1$  respectively. The operator  $\Gamma_5$  is known as the chirality operator, and the spaces of sections of  $S^\pm$  are the right-handed and left-handed fermions respectively. Notice that  $\Gamma_5\psi^\pm = \pm\psi^\pm$ , and the chiral projectors, i.e., the orthogonal projectors into the orthogonal subspaces  $S^\pm$  are given by  $\Pi_\pm = 1/2(I \pm \Gamma_5)$ . Thus given any section  $\psi$  of  $T\Sigma^\mathbb{C}$ , we have  $\psi = \psi^+ + \psi^-$ ,  $\psi^\pm = \Pi_\pm\psi$ . Notice finally that  $[\not{D}, \Gamma_5]_+ = 0$ , where  $[\cdot, \cdot]_+$  denotes the anticommutator, hence  $\not{D}: S^\pm \rightarrow S^\mp$ , and  $\not{D}$  exchanges the irreducible representation spaces as it is apparent from the block structure of the matrix representing  $\not{D}$  above.

Assuming that the boundary is connected, i.e.,  $\partial\Sigma \cong S^1$ , then the space of boundary data  $\mathcal{H}_D$  is given as  $H^{1/2}(S^1, S_{\partial\Omega})$  which is isomorphic to the space of functions of Sobolev class  $1/2$  on  $S^1$  with values in  $\mathbb{C}^2$ . Clifford multiplication by  $\nu$ , the outward normal determines a polarisation  $\mathcal{H}_D = \mathcal{H}_+ \oplus \mathcal{H}_-$  as described in Eq. (13). Thus, according with Thm. 1 the space of self-adjoint extensions of  $\not{D}$  is given by the family of unitary operators  $\mathcal{U}(\mathcal{H}_+, \mathcal{H}_-)$ . Notice that each one of the subspaces  $\mathcal{H}_\pm$  is isomorphic to  $H^{1/2}(S^1)$ , hence the space of self-adjoint extensions can be identified with the group of unitary operators of the Sobolev space  $H^{1/2}(S^1)$ .

### 3. Self-adjoint extensions of Laplace operators

#### 3.1. The covariant Laplacian

We will start the discussion of the theory of self-adjoint extensions of second order differential operators considering a particular situation of big physical interest. Later on, we will extend this considerations to more general families of second order operators and we will find the relation with the theory of extensions for Dirac operators studied in the first part.

We will consider a physical system subject to the action of a Yang–Mills field. The configuration space of the system will be a compact connected smooth Riemannian manifold  $(\Omega, \eta)$  with smooth boundary  $\partial\Omega$ <sup>b</sup>. We will consider a hermitian vector bundle  $E \rightarrow \Omega$  with hermitian product  $(\cdot, \cdot)$ . The Yang–Mills potential will be a connection 1-form  $A$  with values on  $\text{End}(E)$ . The space of smooth sections of  $E$  will be denoted by  $\Gamma(E)$  and the covariant differential operator  $d_A = d + A$  will map  $\Gamma(E)$  to  $\Gamma(E) \otimes \Lambda^1(\Omega)$ , i.e., it will map sections of  $E$  to 1-forms in  $\Omega$  with values on  $E$ .

We will define the  $L^2$ -product  $\langle \cdot, \cdot \rangle$  in  $\Gamma(E)$  as usual,

$$\langle \psi_1, \psi_2 \rangle = \int_{\Omega} (\psi_1(x), \psi_2(x))_x \text{vol}_{\eta}(x), \quad (16)$$

where  $\text{vol}_{\eta}$  denotes the Riemannian volume defined by the metric  $\eta$ . We define  $L^2(E)$  as the completion with respect to the norm  $\| \cdot \|_2$  of the space  $\Gamma(E)$ .

Similarly, we will define the product of two  $k$ -forms  $\alpha, \beta$  on  $\Omega$  with values on  $E$  by the formula,

$$\langle \alpha, \beta \rangle = \int_{\Omega} (\alpha_{i_1 \dots i_k}(x), \beta^{i_1 \dots i_k}(x)) \text{vol}_{\eta}(x),$$

where we have used the metric  $g$  to raise the subindexes on the components of  $\beta$ . We define the Hodge operator  $\star$  as a map from  $\Gamma(E) \otimes \Lambda^k(\Omega)$  to  $\Gamma(E) \otimes \Lambda^{n-k}(\Omega)$ , defined by

$$\star \alpha(x) \wedge \beta(x) = (\alpha_{i_1 \dots i_k}(x), \beta^{i_1 \dots i_k}(x)) \eta_g(x),$$

and thus,

$$\langle \alpha, \beta \rangle = \int_{\Omega} \star \alpha \wedge \beta.$$

We will consider the completion of  $\Gamma(E) \otimes \Lambda^1(\Omega)$  with respect to the norm  $\|\alpha\|_2^2 = \langle \alpha, \alpha \rangle$  and then define the adjoint to the operator  $d_A$  with respect to this Hilbert space structure, i.e.,

$$\langle d_A^\dagger \alpha, \psi \rangle = \langle \alpha, d_A \psi \rangle,$$

for all  $\psi \in \Gamma(E)$  (notice that  $d_A^\dagger$  is well defined because  $\Gamma(E)$  is dense in  $L^2(\Omega, E)$ ).

<sup>b</sup>The theory can be generalized for boundaries with singularities and noncompact manifolds under appropriate regularity conditions



The quantum Hamiltonian for a particle moving in the presence of the Yang–Mills potential  $A$  is formally given by the second order differential operator,

$$\mathbb{H} = -\frac{1}{2}\Delta_A + V, \quad (17)$$

where

$$\Delta_A = d_A^\dagger d_A + d_A d_A^\dagger,$$

is the covariant Laplace–Beltrami operator and  $V$  is a smooth function on  $\Omega$ .

Clearly, the operator  $\Delta_A$  is closable and symmetric on  $\Gamma_0^\infty(E)$ . Its closure is defined on the domain  $H_0^2(\Omega, E)$ , i.e., the completion of  $\Gamma_0^\infty(E)$  with respect to the Sobolev norm  $\|\cdot\|_{2,2}$  defined in Eq. (7) with  $k = 2$ . In fact, such space is the space of sections of  $E$  vanishing on  $\partial\Omega$ , such that they possess first and second weak derivatives which are in  $L^2(\Omega, E)$ . We will denote this operator by  $\Delta_0$ ,  $\text{Dom } \Delta_0 = H_0^2(\Omega, E)$ .

The operator  $\Delta_A$  has another extension, the largest space where it can be defined, the closure of  $\Gamma(E)$  with respect to  $\|\cdot\|_{2,2}$ . This domain is the Sobolev space  $H^2(\Omega, E)$  and it is easy to check that the adjoint of  $\Delta_0$  is precisely  $\Delta_A$  with domain  $H^2(\Omega, E)$ , thus  $\text{Dom } \Delta_0^\dagger = H^2(\Omega, E)$ ,  $\Delta_0^\dagger = \Delta_A$ . On the other hand the smooth function  $V$  defines an essentially self-adjoint operator on  $H^2(\Omega, E)$ . If we denote by  $\mathbb{H}_0$  the operator defined by  $\mathbb{H}$  with domain  $H_0^2(\Omega, E)$  it is possible to check that  $\mathbb{H}_0^\dagger = \mathbb{H}$ , i.e., the domain of the adjoint operator of  $\mathbb{H}_0$  is  $H^2(\Omega, E)$ . Hence, the operator  $\mathbb{H}$  defined on  $H^2(E)$  is not self-adjoint in general. We will be interested in finding extensions  $\mathbb{H}_s$  of  $\mathbb{H}_0$  with domain  $\text{Dom } \mathbb{H}_s$  such that

$$H_0^2(\Omega, E) = \text{Dom } \mathbb{H}_0 \subset \text{Dom } \mathbb{H}_s = \text{Dom } \mathbb{H}_s^\dagger \subset \text{Dom } \mathbb{H} = H^2(\Omega, E),$$

and  $\mathbb{H}_s \psi = \mathbb{H}_0 \psi$ , for any  $\psi \in H_0^2(\Omega, E)$ . To do that, we will integrate by parts as follows.

$$\langle \psi_1, \mathbb{H} \psi_2 \rangle = \langle \mathbb{H} \psi_1, \psi_2 \rangle + \frac{1}{2} \Sigma(\psi_1, \psi_2), \quad (18)$$

for any smooth sections  $\psi_1, \psi_2 \in \Gamma(E)$ , where by Stokes theorem and the parallelism of  $(\cdot, \cdot)$  with respect to the connection defined by  $A$ , we get:

$$\Sigma(\psi_1, \psi_2) = \int_{\partial\Omega} i^*[(\star d_A \psi_1, \psi_2) - (\psi_1, \star d_A \psi_2)]. \quad (19)$$

Notice that  $\star d_A \psi$  is an  $(n-1)$ -form on  $\Omega$  with values in  $E$ , and then  $(\star d_A \psi_1, \psi_2)$  denotes the  $(n-1)$ -form on  $\Omega$  obtained by taking the product of the values of  $\star d_A \psi_1$  and  $\psi_2$  on the fibres of  $E$ .

The boundary term  $\Sigma(\psi_1, \psi_2)$  has a relevant physical interpretation. It measures the net total probability flux across the boundary. If the operator  $\mathbb{H}$  were self-adjoint this flux would have to vanish: the incoming flux would have to be equal to the outgoing flux because the evolution operator  $\exp it\mathbb{H}$  in such a case would be unitary and preserve probability.

We will characterize first self-adjoint extensions of  $\mathbb{H}_0$  by using the geometry of some Hilbert spaces defined on the boundary  $\partial\Omega$  of  $\Omega$  and later on, we will compare with the classical theory of von Neumann.

### 3.2. Complex structures on the Hilbert space of boundary data

We will denote again by  $E_{\partial\Omega}$  the restriction of the bundle  $E$  to  $\partial\Omega$ . Let us denote by  $\text{vol}_{\partial\Omega}$  the Riemannian volume form defined by the restriction  $\partial\eta$  of the Riemannian metric  $\eta$  to the boundary  $\partial\Omega$ . Then we will denote by  $L^2(\Omega, E_{\partial\Omega})$  the Hilbert space of square integrable sections of the bundle  $E_{\partial\Omega}$  and by  $\langle \cdot, \cdot \rangle_{\partial\Omega}$  its Hilbert product structure given by,

$$\langle \psi, \varphi \rangle_{\partial\Omega} = \int_{\partial\Omega} (\psi(x), \varphi(x)) \text{vol}_{\partial\Omega}. \quad (20)$$

To any section  $\Psi \in \Gamma(E)$  we can associate two sections  $\varphi, \dot{\varphi} \in \Gamma(E_{\partial\Omega})$  as follows,

$$\begin{aligned} i^* \Psi &= \varphi \\ i^*(\star d_A \Psi) &= \dot{\varphi} \text{vol}_{\partial\Omega}, \end{aligned} \quad (21)$$

in other words, the function  $\varphi$  is the restriction to  $\partial\Omega$  of  $\Psi$ , and  $\dot{\varphi}$  is the normal derivative of  $\Psi$  along the boundary.

Thus the restriction map  $b: \Gamma(E) \rightarrow \Gamma(E_{\partial\Omega}) \times \Gamma(E_{\partial\Omega})$ , assigning to each section its Dirichlet boundary data,  $\Psi \mapsto b(\Psi) = (\varphi, \dot{\varphi})$ , extends to a continuous linear map,

$$b: H^2(\Omega, E) \rightarrow H^{3/2}(\partial\Omega, E_{\partial\Omega}) \oplus H^{1/2}(\partial\Omega, E_{\partial\Omega}),$$

from the Hilbert space  $H^2(\Omega, E)$  to the direct sum Hilbert space of boundary data  $H^{3/2}(\partial\Omega, E_{\partial\Omega})$  and  $H^{1/2}(\partial\Omega, E_{\partial\Omega})$  equipped with the canonical direct sum product,

$$\langle (\varphi_1, \dot{\varphi}_1), (\varphi_2, \dot{\varphi}_2) \rangle = \langle \varphi_1, \varphi_2 \rangle_{\partial\Omega} + \langle \dot{\varphi}_1, \dot{\varphi}_2 \rangle_{\partial\Omega}. \quad (22)$$

We will call the Hilbert space  $H^{3/2}(\Omega, E_{\partial\Omega}) \oplus H^{1/2}(\Omega, E_{\partial\Omega})$  the Hilbert space of boundary data of the Laplacian operator and we will denote it by  $\mathcal{H}_L$ .

To avoid the difficulties arising from the different spaces contributing as factors to  $\mathcal{H}_L$  we will restrict the second factor to  $H^{3/2}(\partial\Omega, E_{\partial\Omega}) \subset H^{1/2}(\partial\Omega, E_{\partial\Omega})$ , or we imbed both of them into  $L^2(\Omega, E_{\partial\Omega})$ . As it happens with the boundary data space  $\mathcal{H}_D$  for the Dirac operator, the boundary Hilbert space  $\mathcal{H}_L$  has an interesting extra geometrical structure, a canonical compatible complex structure  $J_L$ . Apart from the natural complex structure inherited from  $L^2(\Omega, E_{\partial\Omega})$  there is another complex structure defined by

$$J_L(\varphi, \dot{\varphi}) = (\dot{\varphi}, -\varphi), \quad (23)$$

which clearly is unitary and verifies  $J^\dagger = -J$ . Then the composition with the Hilbert space product defines a skew-pseudo-hermitian product  $\omega_L$  on  $\mathcal{H}_L$ , i.e.,

$$\omega_L((\varphi_1, \dot{\varphi}_1), (\varphi_2, \dot{\varphi}_2)) = \langle J_L(\varphi_1, \dot{\varphi}_1), (\varphi_2, \dot{\varphi}_2) \rangle = \langle \dot{\varphi}_1, \varphi_2 \rangle - \langle \varphi_1, \dot{\varphi}_2 \rangle. \quad (24)$$

For practical purposes it is sometimes convenient to redefine  $\omega_L$  as  $\sigma_L = -\frac{i}{2}\omega_L$ , then  $\sigma_L$  defines a pseudo-Hermitian structure on  $\mathcal{H}_L$ . The skew-pseudo-Hermitian structure  $\omega_L$  defined on the boundary data has been sometimes called the Lagrange form because of Lagrange's identity in the one-dimensional case [Na68].

Then, the boundary term for the Laplace operator obtained in eq. (19) can be simply written as

$$\Sigma(\psi_1, \psi_2) = \omega_L(b(\psi_1), b(\psi_2)),$$

showing explicitly its geometrical nature and allowing a direct characterization of all self-adjoint extensions of  $\mathbb{H}_0$ .

Let  $\mathbb{H}_s$  be a self-adjoint extension of  $\mathbb{H}_0$ . It is obvious that because of Eq. (18),  $b(\text{Dom}(\mathbb{H}_s))$  is a subspace of  $\mathcal{H}_L$  such that  $\omega_L|_{b(\text{Dom}(\mathbb{H}_s))} = 0$ , i.e.,  $b(\text{Dom}(\mathbb{H}_s))$  is an isotropic subspace with respect to the skew-pseudo-hermitian structure  $\omega_L$ .

**Theorem 3.** *There is a one-to-one correspondence between self-adjoint extensions of the operator  $\mathbb{H}_0$  and maximal  $\omega_L$ -isotropic subspaces of  $\mathcal{H}_L$ . Moreover, such self-adjoint extensions are in one-to-one correspondence with self-adjoint subspaces of  $\mathcal{H}_L$  and the eigenspaces of  $J_L$  provide a polarization of the boundary Hilbert space  $\mathcal{H}_L = \mathcal{H}_+ \oplus \mathcal{H}_-$  such that the self-adjoint extensions of  $\mathbb{H}_0$  are in one-to-one correspondence with the unitary operators  $\mathcal{U}(\mathcal{H}_+, \mathcal{H}_-)$ .*

**Proof.** The first part of the theorem is proved very much like Thm. 1. If  $\mathbb{H}'$  is self-adjoint, we have seen that  $b(\mathcal{D}')$  is isotropic. If it were not maximal, this would imply that there is an isotropic subspace  $\mathcal{I}$  that contains properly the domain of  $\mathbb{H}'$ ,  $b(\mathcal{D}') \subset \mathcal{I}$ . Then  $b^{-1}(\mathcal{I})$  is the domain of an extension ( $b$  is continuous) of  $\mathbb{H}_0$  and it verifies

$$\mathcal{D}' \subset b^{-1}(\mathcal{I}) \subset b^{-1}(\mathcal{I}) \subset (\mathcal{D}')^\dagger.$$

In fact, the isotropy of  $\mathcal{I}$  implies that,

$$\langle \psi_1, \mathbb{H}'\psi_2 \rangle = \langle \mathbb{H}'\psi_1, \psi_2 \rangle, \quad \forall \psi_1, \psi_2 \in b^{-1}(\mathcal{I}),$$

because  $\Sigma_B|_{\mathcal{I}} = 0$ .

Conversely, if  $\mathcal{I}$  is a maximal isotropic subspace of  $\mathcal{H}_B$  is evident that the subspace  $b^{-1}(\mathcal{I})$  defines the domain of a self-adjoint extension of  $\mathbb{H}_0$ . In fact, if  $b^{-1}(\mathcal{I}) \subset (b^{-1}(\mathcal{I}))^\dagger$ , then  $b((b^{-1}(\mathcal{I}))^\dagger)$  is an isotropic subspace of  $\mathcal{H}_B$  containing  $\mathcal{I}$ . Thus, because  $\mathcal{I}$  is maximal, they must coincide. Then,  $D_{\mathcal{I}} = b^{-1}(\mathcal{I})$  defines a self-adjoint extension of  $\mathbb{H}_0$ .

Before proving the other statements, we will introduce the analogue of the Cayley transformation discussed in §2.3 for the Laplace operator.  $\square$

### 3.3. The Cayley transformation on the boundary Hilbert space for Laplacian operators

We will concentrate now in the boundary Hilbert space  $\mathcal{H}_L$  with its skew-pseudo-hermitian structure  $\omega_L$ . It is obvious that the subspaces  $\mathcal{L}_+ = L^2(E_{\partial\Omega}) \times \{\mathbf{0}\} = \{(\varphi, \mathbf{0}) \mid \varphi \in L^2(E_{\partial\Omega})\}$  and  $\mathcal{L}_- = \{\mathbf{0}\} \times L^2(E_{\partial\Omega}) = \{(\mathbf{0}, \dot{\varphi}) \mid \dot{\varphi} \in L^2(E_{\partial\Omega})\}$  are isotropic and they paired by  $\omega_L$ . In fact,

$$\omega_L(\varphi_1, \mathbf{0}; \mathbf{0}, \dot{\varphi}_2) = \frac{1}{2} \langle \varphi_1, \dot{\varphi}_2 \rangle_{\partial\Omega}.$$

Thus the block structure of  $\omega_L$  with respect to the isotropic polarization  $\mathcal{H}_L = \mathcal{L}_+ \oplus \mathcal{L}_-$  is

$$\omega_L = \left( \begin{array}{c|c} 0 & \frac{1}{2} \langle \cdot, \cdot \rangle_{\partial\Omega} \\ \hline -\frac{1}{2} \langle \cdot, \cdot \rangle_{\partial\Omega} & 0 \end{array} \right).$$

It will be convenient for further purposes to introduce another pseudo-Hermitian product on  $\mathcal{H}_L$  that corresponds to the diagonalization of  $\omega_L$ , hence of  $J_L$ . We shall define the Cayley transform on the boundary as the map  $C: \mathcal{H}_L \rightarrow \mathcal{H}_L$ , given by,

$$C(\varphi, \dot{\varphi}) = (\varphi + i\dot{\varphi}, \varphi - i\dot{\varphi}), \quad \forall (\varphi, \dot{\varphi}) \in \mathcal{H}_L. \quad (25)$$

We will denote by  $\varphi^\pm = \varphi \pm i\dot{\varphi}$  the components of  $C(\varphi, \dot{\varphi})$ . It is clear that  $C$  is an isomorphism of linear spaces and transforms the pseudo-Hermitian product  $\omega_L$  into the skew-pseudo-hermitian product  $\langle \cdot, \cdot \rangle_{\partial\Omega} \ominus \langle \cdot, \cdot \rangle_{\partial\Omega}$ , i.e.,

$$\sigma_L(\varphi_1^+, \varphi_1^-; \varphi_2^+, \varphi_2^-) = \langle \varphi_1^+, \varphi_2^+ \rangle_{\partial\Omega} - \langle \varphi_1^-, \varphi_2^- \rangle_{\partial\Omega}, \quad \forall (\varphi_a^+, \varphi_a^-) \in \mathcal{H}_L, a = 1, 2. \quad (26)$$

and

$$\omega_L(\varphi_1, \dot{\varphi}_1; \varphi_2, \dot{\varphi}_2) = \sigma_L(\varphi_1^+, \varphi_1^-; \varphi_2^+, \varphi_2^-).$$

Thus, the complex structure  $J_L$  is transformed into diagonal form, i.e.,  $CJ_L C^{-1}(\varphi^+, \varphi^-) = (-i\varphi^+, i\varphi^-)$ , and the eigenspaces of  $J_L$  define a new polarization of  $\mathcal{H}_L = \mathcal{H}_+ \oplus \mathcal{H}_-$ , where  $\mathcal{H}_\pm = \{\varphi \pm i\dot{\varphi} = 0\}$ . Then the previous discussion can be summarized saying that the Cayley transform  $C$  is an pseudounitary transformation among the pseudo-Hermitian spaces  $(\mathcal{H}_L = \mathcal{L}_+ \oplus \mathcal{L}_-, \omega_L)$  and  $(\mathcal{H}_L = \mathcal{H}_+ \oplus \mathcal{H}_-, \sigma_L)$ .

It is obvious that because  $C$  is an isometry between  $\omega_L$  and  $\sigma_L$  it will carry  $\omega_L$ -isotropic subspaces into  $\sigma_L$ -isotropic subspaces. Then the Cayley transform  $C$  induces a homeomorphism between the corresponding spaces of isotropic subspaces with respect to the natural topology in the set of subspaces of  $\mathcal{H}_L$ . We will discuss the topology of such spaces later on.

Now we will continue the proof of Thm. 3 by showing that the set  $\mathcal{M}$  of all closed maximal  $\sigma_L$ -isotropic subspaces of  $\mathcal{H}_L$  can be identified with the group of unitary operators  $\mathcal{U}$  of  $L^2(\partial\Omega, E_{\partial\Omega})$ .

**Proof.** (Cont.) It is a straightforward consequence of the diagonal expressing of the pseudo-Hermitean product  $\Sigma$ . Any maximal linear isotropic subspace  $N$  is transverse to the subspaces  $\mathcal{H}_\pm$ . Thus  $N$  defines a linear operator  $U: \mathcal{H}_+ \rightarrow \mathcal{H}_-$  and

$$N = \{(\varphi^+, U\varphi^+) \in \mathcal{H} \mid \varphi^+ \in \mathcal{H}_+\} = \text{graph} U. \quad (27)$$

It is also an immediate consequence of the isotropy of  $N$  that

$$\langle \varphi_1^+, \varphi_2^+ \rangle_{\partial\Omega} = \langle U\varphi_1^+, U\varphi_2^+ \rangle_{\partial\Omega},$$

and we conclude that  $U$  is an isometry. The maximality of  $N$  implies that  $U$  is an isomorphism. Then we have that  $\mathcal{M} \cong \mathcal{U}(\mathcal{H}_+, \mathcal{H}_-) \cong \mathcal{U}(L^2(\partial\Omega, E_{\partial\Omega}))$  and the identification is continuous because of the continuous embedding of the space of bounded operators on the space of closed subspaces.  $\square$

**Remark 4.** We should warn the reader that in the statement of the previous results, we have replaced the Sobolev spaces  $H^{3/2}(\partial\Omega, E_{\partial\Omega})$  and  $H^{1/2}(\partial\Omega, E_{\partial\Omega})$  by  $L^2(\partial\Omega, E_{\partial\Omega})$ . Even if this is incorrect, there is a natural way of expression the results in this way by using the appropriate theory of Hilbert scales (see [Ca09, Ch. 2.2]). Now it is obvious that with the above characterization the set of self-adjoint extensions of  $\mathbb{H}$  inherits the group structure of the group of unitary operators  $U(L^2(\Omega, E_{\partial\Omega}))$ .

Notice that the domain of the self-adjoint extension of  $\mathbb{H}_0$  defined by  $U$  is the linear subspace of sections  $\psi$  in  $H^2(\Omega, E)$  such that their boundary values  $\varphi, \dot{\varphi}$  satisfy the condition

$$\varphi - i\dot{\varphi} = U(\varphi + i\varphi). \quad (28)$$

We shall denote such subspace by  $\mathcal{D}_U = \{\psi \in \mathcal{D} \mid b(\psi) \in C^{-1}(\text{graph} U)\}$  or equivalently

$$\mathcal{D}_U = \{\psi \in W^2(E) \mid \varphi - i\dot{\varphi} = U(\varphi + i\varphi)\}. \quad (29)$$

Now it is not hard to see that  $\mathcal{M}_L$  is the space of self-adjoint subspaces of  $\mathcal{H}_L$ . If the self-adjoint subspace  $W$  is transverse to the subspace  $\mathcal{L}_\mp$  then, there will exists a self-adjoint operator  $A_\pm: \mathcal{L}_\pm \rightarrow \mathcal{L}_\mp$ , such  $W$  will be the graph of  $A_\pm$  and we will denote it by  $W_{A_\pm}$ . Notice that on the other hand, the self-adjoint subspaces of  $\mathcal{H}_L$  are precisely the closed maximal  $\omega_L$ -isotropic subspaces of  $\mathcal{H}_L$  with respect to the skew-pseudo-hermitian structure  $\omega_L$ .  $\square$

This characterization is very useful because it allows to write the boundary conditions that characterizes the self-adjoint extension of  $\mathbb{H}$  quite easily. If  $A_+$  is a self-adjoint operator in the boundary, then the self-adjoint subspace defining the self-adjoint extension of  $\mathbb{H}$  is given by the space of  $(\varphi, \dot{\varphi})$  such that

$$\dot{\varphi} = A_+\varphi, \quad (30)$$

22 *M. Asorey, A. Iborra, G. Marmo*

and similarly for  $A_-$ , the boundary condition will then be

$$A_- \dot{\varphi} = \varphi. \quad (31)$$

The corresponding unitary operators are obtained by the Cayley transform on the boundary, i.e., the unitary operator  $U_+$  whose graph is the isotropic subspace image by  $C$  of the self-adjoint subspace defined by  $A_+$ ,

$$\varphi - iA_+\varphi = U_+(\varphi + iA_+\varphi), \quad (32)$$

hence,

$$U_+ = \frac{I - iA_+}{I + iA_+},$$

and similarly for  $A_-$ .

$$U_- = \frac{I + iA_-}{I - iA_-}.$$

Conversely if  $U$  is a unitary operator on the boundary, we can define its Cayley transform as the self-adjoint subspace of  $\mathcal{H}_B$  defined by  $C^{-1}N_U$ , i.e., the inverse image by  $C$  of the isotropic subspace defined by  $U$ . It is clear that not always such subspace will be of the form  $W_{A_\pm}$  for some self-adjoint operator. If either  $A_+$  or  $A_-$  exist, it will be given by the formula

$$A_\pm = i \frac{I \pm U}{I \mp U}. \quad (33)$$

It is obvious that  $A_\pm$  will exist if and only if  $\pm 1$  does not belong to the spectrum of  $U$ . Notice that  $A_-$  is the inverse Cayley transform (if it exists) of  $U^\dagger$ .

The previous considerations show that there is a distinguished set of self-adjoint extensions of  $\mathbb{H}$  for which the expression of the boundary conditions defining their domain are not expressible in the simple form given by Eq. (30) or (31). These self-adjoint extensions correspond to the case that  $\pm 1$  is an eigenvalue of the corresponding unitary operator or equivalently that the self-adjoint subspace defined by the unitary operator is not the graph of a self-adjoint operator on the boundary. We will call them the Cayley surfaces of the space of self-adjoint extensions and they can be described equivalently as follows:

$$\mathcal{C}_\pm = \{ U \in \mathcal{U}(L^2(\partial E)) \mid \pm 1 \in \sigma(U) \} = \{ W \in \mathcal{M}_L \mid \dim W \cap \mathcal{L}_\mp > 0 \}. \quad (34)$$

Notice that the unitary operators  $\pm I$  are in the Cayley surfaces  $\mathcal{C}_\pm$  respectively and because of Eq. (32)  $I$  defines Dirichlet boundary conditions:

$$\varphi = 0. \quad (35)$$

Moreover the unitary operator  $-I$  is not in the Cayley surface  $\mathcal{C}_+$  and corresponds to the self-adjoint operator  $A = 0$  because of eq. (33), thus using (30) it defines Neumann boundary conditions

$$\dot{\varphi} = 0. \quad (36)$$

These observations provide us a way to classify all self-adjoint extensions of  $\mathbb{H}$  in those which are not in the Cayley surface and those which are inside. We will proceed later on to perform this analysis.

### 3.4. *Squaring the space of boundary conditions of Dirac operators and boundary conditions for Laplace operators*

In the previous sections we have repeated step by step the theory of self-adjoint extensions of the Hodge Laplacian for Dirac operators. The results are similar but subtly different due to the fundamental different nature of both families of operators.

In both theories a crucial role is played by a skew-pseudo-Hermitean structure on the Hilbert space of boundary data. In fact, the space of self-adjoint extensions is identified with a Lagrangian submanifold of the infinite dimensional Grassmannian naturally defined by such structure. On the other hand, we have already noticed that self-adjoint extensions arise in a twisted way in both cases, i.e., the Cayley transform exchanges unitary and self-adjoint subspaces in reverse order.

On the other hand, Dirac operators  $\mathcal{D}$  lead naturally to elliptic second order differential operators, the Dirac Laplacian  $\mathcal{D}^2$ , which are closely related to Hodge Laplacians by Bochner's identities that play a fundamental role in understanding topological properties of Riemannian manifolds. Such process of squaring a Dirac operator, should lead to a precise link between the theory of self-adjoint extensions of Laplace operators and Dirac operators. We will discuss this link in this section finding out that squaring of Dirac operators has a natural abstract counterpart in the boundary Hilbert spaces of the operators. This construction will be called squaring a Hilbert space with a skew-pseudo-Hermitean structure.

Let  $\mathcal{D}$  denote a Dirac operator on the Dirac bundle  $S \rightarrow \Omega$  and  $\mathcal{H}_D$  the Hilbert space of boundary data for  $\mathcal{D}$  equipped with the canonical compatible complex structure  $J_D$ . We shall consider now the Dirac Laplacian  $\mathcal{D}^2: \Gamma_0(S) \rightarrow \Gamma_0(S)$ . The Dirac Laplacian is obviously a symmetric operator in the domain  $H_0^2(S)$ , which is the closure of  $\Gamma_0(S)$  with respect to the Sobolev norm  $\|\cdot\|_{2,2}$ . Notice that the operator  $\mathcal{D}^2$  with domain  $H_0^2(S)$  is the closure of  $\mathcal{D}^2$  defined on  $\Gamma_0(S)$ . We shall study now the self-adjoint extensions of  $\mathcal{D}^2$ . Then we integrate by parts the  $L^2$ -product  $\langle \mathcal{D}^2 \xi, \zeta \rangle$ ,

$$\begin{aligned} \langle \mathcal{D}^2 \xi, \zeta \rangle &= \langle \mathcal{D} \xi, \mathcal{D} \zeta \rangle + \Sigma(\mathcal{D} \xi, \zeta) \\ &= \langle \xi, \mathcal{D}^2 \zeta \rangle + \Sigma(\xi, \mathcal{D} \zeta) + \Sigma(\mathcal{D} \xi, \zeta), \end{aligned} \quad (37)$$

where we have used the computation in eqs. (11). But because of Eq. (14) we have that,

$$\Sigma(\mathcal{D} \xi, \zeta) = \langle Jb(\mathcal{D} \xi), b(\zeta) \rangle. \quad (38)$$

The effect of the boundary map  $b$  on  $\mathcal{D} \xi$  will be computed as follows. We choose a collar neighborhood  $U_\epsilon$  of the boundary  $\partial\Omega$ . Notice that because  $\partial\Omega$  is compact,

there exists  $\epsilon > 0$  such that the map  $x \mapsto (s, y)$ , with  $y$  the point in  $\partial\Omega$  closest to  $x$  and  $s = \text{dist}(x, y)$  defines a diffeomorphism between  $U_\epsilon$  and  $(-\epsilon, 0] \times \partial\Omega$ . Using the decomposition of the tangent space defined by the previous diffeomorphism we can write  $\not{D}$  on  $U_\epsilon$  as

$$\not{D} = J(\partial_\nu + \not{D}_{\partial\Omega}) \quad (39)$$

where the vector field  $\nu$  on  $U_\epsilon$  is defined by  $\partial/\partial s$ . Notice that when restricted to  $\partial\Omega$ ,  $\nu$  is just the normal vector to the boundary  $\partial\Omega$ . Thus, the covariant derivative in the normal direction is given by partial derivative with respect to this coordinate and is represented by  $\partial_\nu$ . Then, choosing a orthonormal frame in  $U$  with the first vector the extended vector field  $\tilde{\nu}$ , the Dirac operator  $\not{D}$  splits as in Eq. (38). The symbol  $J$  corresponds to Clifford multiplication by  $\tilde{\nu}$  and restricted to  $\partial\Omega$  gives the complex structure  $J_D$ . The operator  $\not{D}_{\partial\Omega}$  is the transversal Dirac operator that restricted to  $\partial\Omega$  is the Dirac operator of the Dirac bundle  $S_{\partial\Omega}$  discussed in §2. Thus,

$$b(\not{D}\xi) = b((J\partial_\nu + \not{D}_{\partial\Omega})\xi) = Jb(\partial_\nu\xi) + \not{D}_{\partial\Omega}b(\xi). \quad (40)$$

Then,

$$\Sigma(\not{D}\xi, \zeta) = \langle J(Jb(\partial_\nu\xi) + \not{D}_{\partial\Omega}b(\xi)), b(\zeta) \rangle = -\langle b(\partial_\nu\xi), b(\zeta) \rangle + \langle J\not{D}_{\partial\Omega}b(\xi), b(\zeta) \rangle. \quad (41)$$

On the other hand, we can compute similarly the last term in the r.h.s. of Eq. (37), and we obtain,

$$\begin{aligned} \Sigma(\xi, \not{D}\zeta) &= \langle Jb(\xi), b(\not{D}\zeta) \rangle = \langle Jb(\xi), Jb(\partial_\nu\zeta) + \not{D}_{\partial\Omega}b(\zeta) \rangle = \\ &= \langle b(\xi), b(\partial_\nu\zeta) \rangle + \langle Jb(\xi), \not{D}_{\partial\Omega}b(\zeta) \rangle. \end{aligned} \quad (42)$$

Collecting the last terms in eqs. (41), (42), we obtain,

$$\begin{aligned} &\langle J\not{D}_{\partial\Omega}b(\xi), b(\zeta) \rangle + \langle Jb(\xi), \not{D}_{\partial\Omega}b(\zeta) \rangle = \\ &\langle J\not{D}_{\partial\Omega}b(\xi), b(\zeta) \rangle + \langle \not{D}_{\partial\Omega}Jb(\xi), b(\zeta) \rangle \\ &= \langle J\not{D}_{\partial\Omega}b(\xi), b(\zeta) \rangle - \langle J\not{D}_{\partial\Omega}b(\xi), b(\zeta) \rangle = 0, \end{aligned}$$

where we have used that  $\not{D}_{\partial\Omega}$  is essentially self-adjoint on the boundaryless manifold  $\partial\Omega$  and the  $J$  anticommutes with  $\not{D}_{\partial\Omega}$ . Denoting  $b(\xi) = \phi$ ,  $b(\partial_\nu\xi) = \dot{\phi}$ ,  $b(\zeta) = \psi$ ,  $b(\partial_\nu\zeta) = \dot{\psi}$ , we finally obtain,

$$\Sigma(\not{D}\xi, \zeta) + \Sigma(\xi, \not{D}\zeta) = \langle \phi, \dot{\psi} \rangle - \langle \dot{\phi}, \psi \rangle,$$

which is exactly the same boundary term we obtained in our analysis of self-adjoint extensions of the Laplace operator. We can abstractly describe the analysis of self-adjoint extensions of the Dirac Laplacian by considering the Hilbert space  $\mathcal{H}_B = \mathcal{H}_D \oplus \mathcal{H}_D$  with the direct sum inner product  $\langle \cdot, \cdot \rangle_B = \langle \cdot, \cdot \rangle \oplus \langle \cdot, \cdot \rangle$  and the compatible complex structure  $J_B$  on  $\mathcal{H}_B$  defined by as in Eq. (23). Notice that  $J_B$  is not the



direct sum of  $J_D \oplus J_D$  which becomes another compatible complex structure on  $\mathcal{H}_B$ . This process is what will be called squaring the boundary data and is summarized in the following table.

$\mathcal{D}$	$\mathcal{D}^2$
$\mathcal{H}_D = \mathcal{H}_+ \oplus \mathcal{H}_-$	$\mathcal{H}_B = \mathcal{H}_D \oplus \mathcal{H}_D$
$\langle \cdot, \cdot \rangle$	$\langle \cdot, \cdot \rangle_B$
$J_D$	$J_B$
$\omega_D$	$B$
$U(\mathcal{H}_+, \mathcal{H}_-)$	$\mathcal{M}_B$
$\mathcal{M}_D$	$U(\mathcal{H}_D, \mathcal{H}_D)$

The previous discussion implies immediately that the self-adjoint extensions of the Dirac Laplacian  $\mathcal{D}^2$  are described in exactly the same terms as the self-adjoint extensions of the Hodge Laplacian described earlier. We will denote as before by  $\mathcal{M}_B$  the self-adjoint Grassmannian of  $\mathcal{D}^2$  which is diffeomorphic to the self-adjoint Grassmannian of  $\nabla$ . Notice that because of Bochner's identity, this was expected in advance. In fact, the Dirac Laplacian  $\mathcal{D}^2$  and the Hodge Laplacian  $\nabla$  differ only on a curvature term that, because is a zero order operator, is self-adjoint, then both theories should agree. We shall discuss other aspects concerned with these facts later on.

It is only natural what is the relation between self-adjoint extensions of  $\mathcal{D}^2$  and self-adjoint extensions of  $D$ . As we know from the previous discussions such extensions are always self-adjoint spaces of the boundary Hilbert space with respect to a skew-pseudo-hermitian structure induced by a compatible complex structure. As we have shown in this section these structures are related by the “square construction”, thereby there must be a definite relation between them.

First we shall study the self-adjoint extensions of  $\mathcal{D}^2$  induced from those of  $\mathcal{D}$ . Let  $W$  be a self-adjoint subspace of  $\mathcal{H}_D = \mathcal{H}_+ \oplus \mathcal{H}_-$ . If  $\mathcal{D}_W$  is self-adjoint, it will be  $\mathcal{D}_W^2$ . Notice that the boundary data for  $\mathcal{D}^2$  are decomposed as  $\phi = \phi_+ + \phi_-$ , and  $\dot{\phi} = \dot{\phi}_+ + \dot{\phi}_-$  where all the factors are mutually orthogonal because of the decomposition

$$\mathcal{H}_L = \mathcal{H}_D \oplus \mathcal{H}_D = (\mathcal{H}_+ \oplus \mathcal{H}_-) \oplus (\mathcal{H}_+ \oplus \mathcal{H}_-). \quad (43)$$

Because  $\mathcal{D}_W$  is self-adjoint we have

$$\langle \mathcal{D}_W^2 \xi, \zeta \rangle = \langle \mathcal{D}_W \xi, \mathcal{D}_W \zeta \rangle + \omega_D(\dot{\phi}, \psi),$$

and the last term in the r.h.s. must vanish for all  $(\dot{\phi}, \psi) \in W_{2,3}$ . Notice that we are identifying  $W \subset \mathcal{H}_D$  with the diagonal subspace  $W_{2,3}$  obtained taking the second and third terms in the decomposition of  $\mathcal{H}_L$  given in Eq. (43). In the same way, repeating the integration by parts, we will obtain that the term  $\omega_D(\phi, \dot{\psi}) = 0$  for all  $(\phi, \dot{\psi}) \in W_{1,4}$ , where  $W_{1,4} = \{(\phi, 0, 0, \dot{\psi}) \in \mathcal{H}_L \mid (\phi, \dot{\psi}) \in W\}$ . Thus, to the

self-adjoint extension  $\mathcal{D}_W$  we associate the self-adjoint extension, still denoted by  $\mathcal{D}_W^2$ , with self-adjoint subspace  $\tilde{W} = W_{2,3} \oplus W_{1,4}$ .

Conversely, it is clear that  $\mathcal{D}^2$  has far more self-adjoint extensions than those defined by self-adjoint subspaces of  $\mathcal{H}_L$  of the form described above  $\tilde{W}$ . However, it is easy to show that if  $\tilde{W}$  defines a self-adjoint extension of  $\mathcal{D}^2$ , i.e.,  $\tilde{W}$  contains the boundary conditions  $(\phi, \dot{\phi})$  that makes  $\mathcal{D}^2$  self-adjoint, then, the subspace of  $\mathcal{H}_D$  defined by the first component, is going to define an extension of  $\mathcal{D}$ . We shall denote by  $\pi_1: \mathcal{H}_L \rightarrow \mathcal{H}_D$  the projection on the first factor. Then, if  $W$  denotes the projected subspace  $\pi_1(\tilde{W})$ , then, we can ask when  $W$  will be self-adjoint.

The characterization of selfadjoint extensions of  $\mathcal{D}^2$  which are induced by those of  $\mathcal{D}$  can be achieved in simple terms. Let us consider the Clifford algebra element  $e_{n+1} = e_1 \cdot e_2 \cdots e_n$  which in even dimensional manifolds is always non-trivial. In odd dimensional manifolds one can consider the non-trivial representation of the Clifford algebra induced from the  $n+1$ -dimensional Clifford algebra and then  $e_{n+1}$  becomes also non-trivial. In both cases due to the special properties of Clifford algebra we have that  $e_{n+1} \cdot e_i + e_i \cdot e_{n+1} = 0$  for any  $i = 1, 2, \dots, n$  and  $e_{n+1} \cdot \nu + \nu \cdot e_{n+1} = 0$ . The selfadjoint extensions of  $\mathcal{D}$  can then be characterized by unitary operators  $U$  of  $H^1(\Omega, S_{\partial\Omega})$  which commute with  $\nu$ . The corresponding domains are given by

$$\mathcal{D}_{\mathcal{D}_U} = \{\psi \in L^2(\Omega, S); P_- \psi|_{S_{\partial\Omega}} = U e_{n+1} P_+ \psi|_{S_{\partial\Omega}}\}, \quad (44)$$

where  $P_{\pm}$  are the projectors  $P_{\pm} = \frac{1}{2}(\mathbb{I} \pm \nu)$ . The domain of the corresponding Dirac Laplacian  $\mathcal{D}_U^2$  is given by the subdomain of  $\mathcal{D}_{\mathcal{D}_U}$  of spinors  $\psi \in \mathcal{D}_{\mathcal{D}_U}$  such that  $\mathcal{D}\psi \in \mathcal{D}_{\mathcal{D}_U}$ . This requirement imposes further constraints on the normal derivative,

$$\begin{aligned} \mathcal{D}_{\mathcal{D}_U^2} &= \{\psi \in H^2(S); P_- \psi|_{S_{\partial\Omega}} = U e_{n+1} P_+ \psi|_{S_{\partial\Omega}}, \\ &\quad P_- (\mathbb{I} + U e_{n+1}) \partial_{\nu} \psi|_{S_{\partial\Omega}} = P_- (\mathbb{I} - U e_{n+1}) \mathcal{D}_{S_{\partial\Omega}} \psi|_{S_{\partial\Omega}}\} \end{aligned} \quad (45)$$

as required by the boundary conditions of the second order differential operator  $\mathcal{D}^2$  which give rise to selfadjoint extensions. Notice, that these boundary conditions are not the most general ones that make  $\mathcal{D}^2$  selfadjoint, but are the only ones which guarantee that  $\mathcal{D}^2$  is the square of the selfadjoint Dirac operator  $\mathcal{D}$ . To illustrate this let us consider a couple of examples. Let  $U$  be of the form

$$U = e^{2i \arctan e^{\alpha} \nu}, \quad (46)$$

which because of the identities

$$\begin{aligned} \frac{I - U e_{n+1}}{I + U e_{n+1}} &= \frac{I + U}{I - U} (1 - e_{n+1}) + \frac{I - U}{I + U} (1 + e_{n+1}) \\ &= i \cot(\arctan e^{\alpha}) (1 - e_{n+1}) - i \tan(\arctan e^{\alpha}) (1 + e_{n+1}) \\ &= i e^{-\alpha} (1 - e_{n+1}) - i e^{\alpha} (1 + e_{n+1}) = -i e^{\alpha e_{n+1}} e_{n+1}, \end{aligned}$$

corresponds to the chiral bag boundary conditions:

$$\frac{1}{2} (1 - i e_{n+1} e^{-\alpha e_{n+1}} \nu) \psi = 0. \quad (47)$$

In the massive case these extensions can give rise to the existence of edge states [As13, As15]. Another example corresponds to the Atiyah-Patodi-Singer boundary conditions [At75] which are given by  $P_+\psi|_{S_{\partial\Omega}} = 0$ , where  $P_+$  is the orthogonal projector on the subspace of  $H^1(\Omega, S_{\partial\Omega})$  corresponding to the positive spectrum of the selfadjoint operator  $\not{D}_{S_{\partial\Omega}}$  (see later on Sect. 6.1). In that case the spinors of the domain of  $\not{D}^2$  must satisfy the extra requirement that also involves the normal derivative

$$\mathcal{D}_{\not{D}^2} = \{\psi \in H^2(S); P_+\psi|_{S_{\partial\Omega}} = 0, P_+\partial_\nu\psi = -P_+\not{D}_{S_{\partial\Omega}}\psi\}. \quad (48)$$

#### 4. Von Neumann's theorem and boundary conditions revisited

##### 4.1. Von Neumann's theorem vs. unitary operators at the boundary

A theory of self-adjoint extensions of symmetric differential operators based on the geometrical structures induced by them in the corresponding spaces of boundary data has been sketched along the previous sections. However a general solution to this problem was set up by von Neumann [Ne29] in the abstract realm of symmetric operators with dense domains in Hilbert spaces.

We will show the exact nature of the link between both approaches, the one discussed in this work based on geometrical boundary data and von Neumann's based on global information on the bulk.

We have already mentioned the fact that the theory of extensions for the Dirac Laplacian and the covariant Laplacian are the same because Bochner's identity ([La89], Thm. II.8.2) implies that the difference between both operators is a zeroth order operator. Hence we will keep the discussion in this section to the covariant Laplacian without loss of generality.

We have characterized self-adjoint extensions of the covariant Laplacian as unitary operators  $\mathcal{U}(\mathcal{H}_+, \mathcal{H}_-)$  whereas the standard characterization of self-adjoint extensions provided by von Neumann's theorem [Ne29] is by means of unitary operators  $K: \mathcal{N}_i \rightarrow \mathcal{N}_{-i}$  between the deficiency subspaces  $\mathcal{N}_{\pm i} = \{\psi \in L^2(\Omega) \mid \mathbb{H}_0^\dagger \psi = \pm i\psi\}$ . As we have stressed before, the advantage of the former characterization is that it is directly related to conditions that the wave functions must satisfy on the boundary  $\partial\Omega$ .

Before we shall discuss the exact relation between von Neumann's theory and Thm. 3 we should mention that there has been several refinements of von Neumann's theory extending it to more general situations. For instance, if  $*$  denotes a conjugation on a Hilbert space, i.e., an antilinear involution such that  $\langle \psi_1^*, \psi_2^* \rangle = \langle \psi_2, \psi_1 \rangle$ , a linear operator  $A$  with dense domain is said to be  $*$ -symmetric if  $*A^* \subset A^\dagger$ . If  $*A^* = A^\dagger$ , then  $A$  is called  $*$ -self-adjoint. If  $A$  is  $*$ -real, i.e.,  $*A^* = A$ , then  $A$   $*$ -self-adjoint implies that  $A$  is self-adjoint in the standard sense. Then it was proved in [Ga62] that any  $*$ -symmetric operator with dense domain has a  $*$ -self-adjoint extension.

There is also a generalization of von Neumann's theory of extensions of symmetric operators with dense domain to formally normal operators with non-dense domains [Co73]. Both generalizations can be discussed from the viewpoint of the geometry of boundary conditions. We will not insist on this and we will restrict for clarity to the simpler case of self-adjoint extensions of symmetric operators with dense domains.

We denote as usual by  $-\Delta_A^\dagger$  the adjoint, with domain  $\mathcal{D}_{\max} = H^2(E)$ , of the Laplacian  $-\Delta_A$  with domain  $\mathcal{D}_{\min} = H_0^2(E)$ . We will also use the notation  $\mathcal{D}_0$  for the domain  $\mathcal{D}_{\min}$ . Given any  $\lambda \in \mathbb{C}$ ,  $\text{Im}\lambda > 0$ , we define the deficiency spaces  $\mathcal{N}_\lambda$ ,  $\mathcal{N}_{\bar{\lambda}}$ , by,

$$\mathcal{N}_\lambda = \text{Ran}(-\Delta_A + \lambda I)^\perp = \ker(-\Delta_A^\dagger + \bar{\lambda}I), \quad (49)$$

$$\mathcal{N}_{\bar{\lambda}} = \text{Ran}(-\Delta_A + \bar{\lambda}I)^\perp = \ker(-\Delta_A^\dagger + \lambda I), \quad (50)$$

that are closed spaces of the Hilbert space  $L^2(\Omega, E)$ .

It is then true that for any nonreal  $\lambda$ ,

$$\mathcal{D}_{\max} = \mathcal{D}_{\min} + \mathcal{N}_\lambda + \mathcal{N}_{\bar{\lambda}}, \quad (51)$$

and the sum is direct as vector spaces. Von Neumann's theorem states that:

**Theorem 5.** [Ne29] *There exists a one-to-one correspondence between self-adjoint extensions of  $-\Delta_A$  and unitary operators  $K$  from  $\mathcal{N}_\lambda$  to  $\mathcal{N}_{\bar{\lambda}}$ , for any  $\lambda \in \mathbb{C}$ ,  $\text{Im}\lambda > 0$ .*

The domain of the self-adjoint extension corresponding to the operator  $K$  is  $\mathcal{D}_0 + \text{Ran}(I + K)$  and is defined for a function of the form  $\Psi = \Psi_0 + (I + K)\xi_+$ ,  $\Psi_0 \in \mathcal{D}_0$ ,  $\xi_+ \in \mathcal{N}_\lambda$ , by

$$\Delta_A^K \psi = \Delta_A \Psi_0 + \bar{\lambda} \xi_+ + \lambda K \xi_+.$$

Notice that the theorem implies that all deficiency spaces  $\mathcal{N}_\lambda$  with  $\text{Im}\lambda > 0$  are isomorphic.

Different presentations of this theorem, and of Eq. (51), can be found for instance in [Du63], [Ak63], [Na68] [Yo65], [Re75] and [We80] and, as it was already expressed in the introduction, there exists an abundant literature on the subject.

Once that Eq. (51) is established, the main idea of the proof is to show that there is a one-to-one correspondence between extensions of the symmetric operator  $-\Delta_A$  and extensions of its Cayley transform  $U_\Delta: \text{Ran}(-\Delta_A + \bar{\lambda}I) \rightarrow \text{Ran}(-\Delta_A + \lambda I)$  defined by

$$U = \frac{-\Delta_A + \lambda I}{-\Delta_A + \bar{\lambda}I}.$$

To compare with our previous results it will be convenient to describe von Neumann extension theorem in the setting of skew-Hermitian spaces.

We define the total Hilbert deficiency space  $\mathcal{N} = \mathcal{N}_\lambda \oplus \mathcal{N}_{\bar{\lambda}}$ . Similarly to the results obtained in Sections 3.2, 3.3, unitary operators from  $K: \mathcal{N}_\lambda \rightarrow \mathcal{N}_{\bar{\lambda}}$  are in

one-to-one correspondence with maximal isotropic subspaces of  $\mathcal{N}$  with respect to the natural pseudo-Hermitian structure  $\omega_{\mathcal{N}}$  defined on  $\mathcal{N}$  by:

$$\sigma_{\mathcal{N}}((\Psi_1^+, \Psi_1^-), (\Psi_2^+, \Psi_2^-)) = \langle \Psi_1^+, \Psi_2^+ \rangle - \langle \Psi_1^-, \Psi_2^- \rangle, \quad (52)$$

for all  $\Psi_{\alpha}^+ \in \mathcal{N}_{\lambda}, \Psi_{\alpha}^- \in \mathcal{N}_{\bar{\lambda}}, \alpha = 1, 2$ . Now we can try to identify the deficiency space in the bulk  $\mathcal{H}_{VN}$  with the boundary space  $\mathcal{H}_L$ .

The boundary map  $b$  restricts to  $\mathcal{N} \subset H^2(E)$ , and moreover  $b$  restricts to the closed subspaces  $\mathcal{N}_{\lambda}, \mathcal{N}_{\bar{\lambda}}$ . We compose  $b$  with the Cayley transform on the boundary  $C$  to obtain a continuous linear map  $j: \mathcal{N} \rightarrow \mathcal{H}_L$  defined as follows. Let  $j_{\pm}(\Psi^{\pm}) = \varphi \pm i\dot{\varphi}$ , where  $(\varphi, \dot{\varphi}) = b(\Psi)$ , where  $j_{\pm}$  denote the restriction of  $j$  to  $\mathcal{N}_{\pm}$  respectively. Then,  $j = j_+ \oplus j_-$ . We will denote  $j_{\pm}(\Psi^{\pm})$  as usual by  $\phi^{\pm}$ . Then,

$$j(\Psi^+, \Psi^-) = (\phi^+, \phi^-). \quad (53)$$

The following Lemma will show that  $j$  preserves the skew-Hermitian structures.

**Lemma 6.** *With the above notation the map  $j: \mathcal{N} \rightarrow \mathcal{H}_L$  verifies*

$$\sigma_{\mathcal{N}}((\Psi_1^+, \Psi_1^-), (\Psi_2^+, \Psi_2^-)) = \sigma_L((\varphi_1^+, \varphi_1^-), (\phi_2^+, \phi_2^-)).$$

*Proof:* We consider  $\lambda = i$ , the proof for general  $\lambda$  proceeds in the same way. We consider first  $\Psi_1^+, \Psi_2^+ \in \mathcal{N}_i$ , then  $-\Delta_A^{\dagger} \Psi_{\alpha}^+ = i\Psi_{\alpha}^+, \alpha = 1, 2$ .

Then it is clear that,

$$\begin{aligned} 0 &= \langle \Psi_1^+, (-\Delta_A^{\dagger} - i)\Psi_2^+ \rangle = \langle \Psi_1^+, -\Delta_A \Psi_2^+ \rangle - i\langle \Psi_1^+, \Psi_2^+ \rangle \\ &= \langle -\Delta_A \Psi_1^+, \Psi_2^+ \rangle - i\Sigma_B(b(\Psi_1^+), b(\Psi_2^+)) - i\langle \Psi_1^+, \Psi_2^+ \rangle \\ &= \langle (-\Delta_A - i)\Psi_1^+, \Psi_2^+ \rangle - 2i\langle \Psi_1^+, \Psi_2^+ \rangle - i\Sigma_B(\phi_1^+, \phi_2^+) \\ &= -2i\langle \Psi_1^+, \Psi_2^+ \rangle - i\Sigma_B(\phi_1^+, \phi_2^+). \end{aligned}$$

Hence,

$$\sigma_{\mathcal{N}}((\Psi_1^+, 0), (\Psi_2^+, 0)) = \langle \Psi_1^+, \Psi_2^+ \rangle = -\frac{1}{2}\sigma_L(\phi_1^+, \phi_2^+) = -\frac{1}{2}\sigma(\phi_1^+, 0; \phi_2^+, 0).$$

Similarly, it is shown,

$$\sigma_{\mathcal{N}}(0, \Psi_1^-, 0, \Psi_2^-) = \sigma(0, \phi_1^-; 0, \phi_2^-),$$

that together with the ortogonality of  $\mathcal{N}_i$  and  $\mathcal{N}_{-i}$  with respect to  $\sigma_L$  proves the result.  $\square$

To show that  $j$  is onto we will need the following facts from the existence and uniqueness of solutions of the following Dirichlet's problem.

**Proposition 7.** *For every  $\varphi \in \Gamma^{\infty}(\partial E)$ , and for every  $\lambda \in \mathbb{C}$  there is a unique solution to the equations,*

$$-\Delta_A \Psi + \bar{\lambda} \Psi = 0, \quad -\Delta_A \Psi + \lambda \Psi = 0, \quad (54)$$

30 *M. Asorey, A. Ibort, G. Marmo*

with boundary condition

$$\Psi|_{\partial\Omega} = \varphi.$$

**Proof.** We prove first uniqueness. If there were two solutions  $\Psi_1, \Psi_2$ , then because the operator  $-\Delta_A + \bar{\lambda}$  is elliptic, then because  $\varphi$  is smooth, by elliptic regularity they will be both smooth. Then,  $\Psi = \Psi_1 - \Psi_2$  also satisfies Eq. (54) with the boundary condition  $\Psi|_{\partial\Omega} = 0$ , which is impossible by the uniqueness of the solution of the Dirichlet's problem. Moreover we can argue as follows. If we look for solutions  $\Psi$  of the equation (54) such that  $\Psi|_{\partial\Omega} = \text{constant}$ , then, we can remove the boundary identifying all their points and looking for the solutions of eq. (54) on the closed manifold  $\Omega'$  obtained in this way. But now,  $-\Delta_A$  is essentially self-adjoint on  $\Gamma(E')$  where  $E'$  is the fibre bundle obtained from  $E$  identifying all the fibres over  $\partial\Omega^c$ , and then it has not imaginary eigenvalues.

Let us now prove the existence of solutions. Let  $\tilde{\Psi}$  be any section in  $\Gamma^\infty(E)$  such that  $\tilde{\Psi}|_{\partial\Omega} = \varphi$ . Then, there exists a unique section  $\zeta \in \Gamma(\Omega)$  such that

$$-\Delta_A \zeta + \bar{\lambda} \zeta = \Delta_A \tilde{\Psi} - \lambda \tilde{\Psi},$$

with Dirichlet boundary conditions,  $\zeta|_{\partial\Omega} = 0$  which is a consequence of the solution of the Dirichlet boundary value problem for elliptic operators. Then, the section  $\Psi = \zeta + \tilde{\Psi}$  verifies Eq. (54) and the boundary condition  $\Psi|_{\partial\Omega} = \varphi$ .  $\square$

Notice that because of Lions' Theorem [Li72] the previous theorem can be refined assuming that  $\varphi \in H^{3/2}(\partial\Omega)$ . In that case the solution  $\Psi$  will lie in  $H^2(\Omega)$ .

An alternative argument to the previous proof will be to consider the operator  $T = (-\Delta_A + \bar{\lambda})(-\Delta_A + \lambda) = \Delta^2 - 2\text{Re}\lambda\Delta + |\lambda|^2$  which is a positive 4th order elliptic differential operator and solve the equation  $T\Psi = 0$  with boundary conditions  $\Psi|_{\partial\Omega} = \varphi$ , and  $([-\Delta_A + \lambda]\Psi)|_{\partial\Omega} = 0$  which are elliptic boundary conditions. Hence there is a unique solution to the system  $\Psi$  which obviously solves the system Eq. (54).

**Theorem 8.** *The total deficiency space on the bulk  $\mathcal{N}$  with its natural skew-Hermitean structure  $\sigma_{\mathcal{N}}$  is isometrically isomorphic to the boundary data space  $\mathcal{H}_L$  with its natural skew-Hermitean structure  $\sigma_L$  as skew-Hermitean spaces.*

**Proof.** We will have to show that the map  $j$  is onto. We can solve the boundary problems

$$-\Delta_A \Psi^+ + \bar{\lambda} \Psi^+ = 0, \quad \Psi^+|_{\partial\Omega} = \phi^+ \quad (55)$$

$$-\Delta_A \Psi^- + \bar{\lambda} \Psi^- = 0, \quad \Psi^-|_{\partial\Omega} = \phi^-, \quad (56)$$

for given  $(\phi^+, \phi^-) \in \Gamma^\infty(\partial\Omega \times \partial\Omega)$ . notice that such solutions will lie necessarily on  $\mathcal{N}_\lambda, \mathcal{N}_{\bar{\lambda}}$ . Proposition 7 shows that such solutions  $\Psi^+, \Psi^-$  exist and they are unique.

<sup>c</sup>Notice that the compactness of  $\Omega$  is crucial in this statement.

They define the inverse of the map  $j$  on the dense subspace  $\Gamma^\infty(\partial\Omega \times \partial\Omega)$ , and it is continuous as the resolvents of the operators  $-\Delta_A + \bar{\lambda}$ ,  $-\Delta_A + \lambda$  are compact. Thus  $j$  is an isometry onto.  $\square$

The following result follows immediately from the previous discussion.

**Corollary 9.** *There is a one-to-one correspondence  $K \mapsto U$  between unitary operators  $K$  from  $\mathcal{N}_\lambda$  to  $\mathcal{N}_{\bar{\lambda}}$  and unitary operators  $U$  at the boundary given as:*

$$\text{graph}(U) = b(\text{graph}(K)),$$

or, in other words,

$$U = b \circ K \circ j. \quad (57)$$

**Remark 10.** A few remarks concerning the previous results are in order.

- (1) Notice first that the previous theorem can also be seen as offering an alternative proof of von Neumann's theorem.
- (2) The previous statement could also be expressed in terms of the “direct” boundary data  $\varphi$  and  $\dot{\varphi}$ . In fact they will be obtained from the expressions:

$$\varphi = \frac{1}{2}(\phi^+ + \phi^-); \quad \dot{\varphi} = -\frac{i}{2}(\phi^+ - \phi^-).$$

- (3) The previous correspondence between unitary operators can be extended to any operator  $L: \mathcal{N}_+ \rightarrow \mathcal{N}_-$  not necessarily unitary by means of formula Eq. (57), that is given the (non-unitary) operator  $L$  we define the (non-unitary) operator from  $\mathcal{H}_+$  to  $\mathcal{H}_-$ :

$$A = b \circ L \circ j.$$

This fact will be of consequence later on in Sect. 7 when discussing dissipative quantum systems and non-self-adjoint boundary conditions.

- (4) Notice that Thm. 8 was stated in a way that the specific form of the operator  $\mathbb{H}$  was not appearing explicitly so that it suggests the form that they would have in general. For instance, we can use the results obtained so far to prove the analogue of Thm. 9 for the Dirac operator.

#### 4.2. Examples and applications: Boundary conditions for the Laplace operator in one-dimension

The relation with the classical boundary conditions analyzed in the previous section becomes also clear in the light of this geometric approach. The quantum extension which corresponds to the quantization of the classical boundary condition  $S_\alpha^\rho$  is precisely the one associated to the unitary operator given by

$$U\varphi(x) = \varphi(\rho^{-1}(x))e^{i\alpha(x)} \quad (58)$$

$$\dot{\varphi}(x) = -\dot{\varphi}(\rho^{-1}(x))e^{i\alpha(x)}. \quad (59)$$

We remark, however, there are many other quantum extensions given by operators which are not of the form (58). Therefore, not all constrained quantum systems correspond to the quantization of a constrained classical system.

To illustrate the utility of the above geometric approach we consider some simple applications to Sturm-Liouville problems. In such a case the configuration space is constrained to an interval  $\Omega = [0, 1]$  of real numbers. The metric  $g$  is the standard Euclidean metric of  $\mathbb{R}$  and the symmetric operator is the Sturm-Liouville second order differential operator

$$\mathbb{H} = -\frac{1}{2}\Delta = -\frac{1}{2}\frac{d}{dx^2},$$

defined on  $C_0^\infty([0, 1])$ . The boundary set is in this case discrete:  $\partial\Omega = \{0, 1\}$ , and  $L^2(\partial\Omega) = \mathbb{C}^2$ . Therefore the different self-adjoint extensions are parametrized by a  $2 \times 2$  unitary matrix.

$$U = \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix}. \quad (60)$$

The domain of the associated extension is given by the functions of  $H^2([0, 1])$  whose boundary values satisfy the following equations (notice that we are in a 1-dimensional manifold, and because of Sobolev inequalities, the functions in  $H^2([0, 1])$  are  $C^1$  and their derivatives absolutely continuous):

$$\begin{pmatrix} \varphi(0) + i\dot{\varphi}(0) \\ \varphi(1) + i\dot{\varphi}(1) \end{pmatrix} = \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix} \begin{pmatrix} \varphi(0) - i\dot{\varphi}(0) \\ \varphi(1) - i\dot{\varphi}(1) \end{pmatrix}, \quad (61)$$

where  $\dot{\varphi}(0) = \varphi'(0)$  and  $\dot{\varphi}(1) = -\varphi'(1)$ .

Some specially interesting examples correspond to the case when the matrix  $U$  is diagonal or antidiagonal. In the first case we have

$$U = \begin{pmatrix} e^{i\epsilon} & 0 \\ 0 & e^{-i\gamma} \end{pmatrix}, \quad (62)$$

which corresponds to the boundary conditions

$$-\sin \frac{\epsilon}{2} \varphi(0) + \cos \frac{\epsilon}{2} \dot{\varphi}(0) = 0 \quad (63)$$

$$-\sin \frac{\gamma}{2} \varphi(1) + \cos \frac{\gamma}{2} \dot{\varphi}(1) = 0, \quad (64)$$

which includes Neumann  $\dot{\varphi}(0) = \dot{\varphi}(1) = 0$  and Dirichlet  $\varphi(0) = \varphi(1) = 0$  boundary conditions. In the antidiagonal case

$$U = \begin{pmatrix} 0 & e^{-i\epsilon} \\ e^{i\epsilon} & 0 \end{pmatrix} \quad (65)$$

we have (pseudo-)periodic boundary conditions

$$\varphi(1) = e^{i\epsilon} \varphi(0) \quad (66)$$

$$\dot{\varphi}(1) = e^{i\epsilon} \dot{\varphi}(0) \quad (67)$$

$\varphi(1) = e^{i\epsilon} \varphi(0)$  with probability flux propagating through the boundary.



## 4.2.1. Self-adjoint extensions of Schrödinger operators in 1D

We will concentrate our attention in 1D where we will be able to provide an elegant formula to solve the spectral problem for each self-adjoint extension.

Notice first that a compact 1D manifold  $\Omega$  consists of a finite number of closed intervals  $I_\alpha$ ,  $\alpha = 1, \dots, n$ ,  $x_\alpha \in I_\alpha$  denoting the variable on each one of them. Each interval will have the form  $I_\alpha = [a_\alpha, b_\alpha] \subset \mathbb{R}$  and the boundary of the manifold  $\Omega = \sqcup_{\alpha=1}^n [a_\alpha, b_\alpha]$  (disjoint union) is given by the family of points  $\{a_1, b_1, \dots, a_n, b_n\}$ . Functions  $\Psi$  on  $\Omega$  are determined by vectors  $(\Psi_1(x_1), \dots, \Psi_n(x_n))$  of complex valued functions  $\Psi_\alpha: I_\alpha \rightarrow \mathbb{C}$ .

A Riemannian metric  $\eta$  on  $\Omega$  is given by specifying a Riemannian metric  $\eta_\alpha$  on each interval  $I_\alpha$ , this is, by a positive smooth function  $\eta_\alpha(x_\alpha) > 0$  on the interval  $I_\alpha$ , i.e.,  $\eta|_{I_\alpha} = \eta_\alpha(x_\alpha)dx_\alpha^2$ . Then the inner product on  $I_\alpha$  takes the form  $\langle \Psi_\alpha, \Phi_\alpha \rangle = \int_{a_\alpha}^{b_\alpha} \bar{\Psi}_\alpha(x_\alpha)\Phi_\alpha(x_\alpha)\sqrt{\eta_\alpha(x_\alpha)}dx_\alpha$  and the Hilbert space of square integrable functions on  $\Omega$  is given by  $L^2(\Omega) = \bigoplus_{\alpha=1}^n L^2(I_\alpha, \eta_\alpha)$ . Thus the Hilbert space  $L^2(\partial\Omega)$  at the boundary reduces to  $\mathbb{C}^{2n}$ , as well as the subspaces  $H^{3/2}(\partial\Omega)$  and  $H^{1/2}(\partial\Omega)$ . The vectors in  $L^2(\partial\Omega)$  are determined by the values of  $\Psi$  at the points  $a_\alpha, b_\alpha$  (with the standard inner product):

$$\psi = (\Psi_1(a_1), \Psi_1(b_1), \dots, \Psi_n(a_n), \Psi_n(b_n)).$$

Similarly we will denote by  $\dot{\psi}$  the vector containing the normal derivatives of  $\Psi$  at the boundary, this is:

$$\dot{\psi} = \left( -\frac{d\Psi_1}{dx}\Big|_{a_1}, \frac{d\Psi_1}{dx}\Big|_{b_1}, \dots, -\frac{d\Psi_n}{dx}\Big|_{a_n}, \frac{d\Psi_n}{dx}\Big|_{b_n} \right).$$

Because of Thm. 3 an arbitrary self-adjoint extension of the Schrödinger operator

$$\mathbb{H} = -\frac{1}{2} \bigoplus_{\alpha} \frac{d^2}{dx_\alpha^2} + V(x_1, \dots, x_n),$$

defined by the Riemannian metric  $\eta$  and a regular potential function  $V$  is defined by a unitary operator  $V: \mathbb{C}^{2n} \rightarrow \mathbb{C}^{2n}$ . Its domain consists of those functions whose boundary values  $\psi, \dot{\psi}$  satisfy Asorey's condition, Eq. (28). This equation becomes a finite dimensional linear system for the components of the vectors  $\psi$  and  $\dot{\psi}$ . Hence the space of self-adjoint extensions is in one-to-one correspondence with the unitary group  $U(2n)$  and has dimension  $4n^2$ .

It will be convenient for further purposes to organize the boundary data vectors  $\psi$  and  $\dot{\psi}$  in a different way. Thus, we denote by  $\psi_l \in \mathbb{C}^n$  (respec.  $\psi_r$ ) the column vector whose components  $\psi_l(\alpha)$ ,  $\alpha = 1, \dots, n$ , are the values of  $\Psi$  at the left endpoints  $a_\alpha$ , this is  $\psi_l(\alpha) = \Psi_\alpha(a_\alpha)$  (respec.  $\psi_r(\alpha) = \Psi_\alpha(b_\alpha)$  are the values of  $\Psi$  at the right endpoints). Similarly we will denote by  $\dot{\psi}_l(\alpha) = -\frac{d\Psi_\alpha}{dx}\Big|_{a_\alpha}$  and  $\dot{\psi}_r(\alpha) = \frac{d\Psi_\alpha}{dx}\Big|_{b_\alpha}$ ,  $\alpha = 1, \dots, n$ . Hence, the domain of the self-adjoint extension

defined by the unitary matrix  $U$  will be written accordingly as:

$$\begin{aligned}\psi_l - i\dot{\psi}_l &= U^{11}(\psi_l + i\dot{\psi}_l) + U^{12}(\psi_r + i\dot{\psi}_r) \\ \psi_r - i\dot{\psi}_r &= U^{21}(\psi_l + i\dot{\psi}_l) + U^{22}(\psi_r + i\dot{\psi}_r)\end{aligned}\quad (68)$$

and  $U$  has the block structure:

$$U = \begin{bmatrix} U^{11} & U^{12} \\ U^{21} & U^{22} \end{bmatrix}. \quad (69)$$

Notice that the unitary matrix  $U$  is related to the unitary matrix  $V$  above by a permutation, but we will not need its explicit expression here.

Thus in what follows we will use the notation for the boundary data:

$$\psi = \begin{bmatrix} \psi_l \\ \psi_r \end{bmatrix}; \quad \dot{\psi} = \begin{bmatrix} \dot{\psi}_l \\ \dot{\psi}_r \end{bmatrix}$$

and Asorey's condition reads again:

$$\psi - i\dot{\psi} = U(\psi + i\dot{\psi}), \quad U \in U(2n). \quad (70)$$

#### 4.2.2. The spectral function

Once we have determined a self-adjoint extension  $H_U$  of the Schrödinger operator  $H$ , we can determine the unitary evolution of the system by computing the flow  $U_t = \exp(-itH_U/\hbar)$ . It is well-known that the Dirichlet extension of the Laplace–Beltrami operator has a pure discrete spectrum because of the compactness of the manifold and the ellipticity of the operator, hence all self-adjoint extensions have a pure discrete spectrum (see [We80], Thm. 8.18). Then the spectral theorem for the self-adjoint operator  $H_U$  states:

$$H_U = \sum_{k=1}^{\infty} \lambda_k P_k,$$

where  $P_k$  is the orthogonal projector onto the finite-dimensional eigenvector space  $V_k$  corresponding to the eigenvalue  $\lambda_k$ . The unitary flow  $U_t$  is given by:

$$U_t = \sum_{k=1}^{\infty} e^{-it\lambda_k/\hbar} P_k.$$

Hence all that remains to be done is to solve the eigenvalue problem:

$$H_U \Psi = \lambda \Psi, \quad (71)$$

for the Schrödinger operator  $H_U$ . We devote the rest of this section to provide an explicit formula to solve Eq. (71).

On each subinterval  $I_\alpha = [a_\alpha, b_\alpha]$  the differential operator  $H_\alpha = H|_{I_\alpha}$  takes the form of a Sturm–Liouville operator

$$H_\alpha = -\frac{1}{W_\alpha} \frac{d}{dx} p_\alpha(x) \frac{d}{dx} + V_\alpha(x),$$

with smooth coefficients  $W_\alpha = \frac{1}{2\sqrt{\eta_\alpha}} > 0$  (now and in what follows we are taking the physical constants  $\hbar$  and  $m$  equal to 1),  $p_\alpha(x) = \frac{1}{\sqrt{\eta_\alpha}}$ , hence the second order differential equation

$$H_\alpha \Psi_\alpha = \lambda \Psi_\alpha \quad (72)$$

has a two-dimensional linear space of solutions for each  $\lambda$ . We shall denote a basis of solutions of such space as  $\Psi_\alpha^\sigma$ ,  $\sigma = 1, 2$ . Notice that  $\Psi_\alpha^\sigma$  depends differentially on  $\lambda$ . Hence a generic solution of Eq. (72) takes the form:

$$\Psi_\alpha = A_{\alpha,1} \Psi_\alpha^1 + A_{\alpha,2} \Psi_\alpha^2.$$

Now it is clear that

$$\psi_l(\alpha) = \Psi_\alpha(a_\alpha) = A_{\alpha,1} \psi_a^1(\alpha) + A_{\alpha,2} \psi_a^2(\alpha).$$

Hence:

$$\psi_l = A_1 \circ \psi_a^1 + A_2 \circ \psi_a^2,$$

where  $A_\sigma$ ,  $\sigma = 1, 2$ , denotes the column vector

$$A_\sigma = \begin{bmatrix} A_{1,\sigma} \\ \vdots \\ A_{n,\sigma} \end{bmatrix}$$

and  $\circ$  denotes the Hadamard product of two vectors, i.e.,  $(X \circ Y)_\alpha = X_\alpha Y_\alpha$  where  $X, Y \in \mathbb{C}^n$ . We obtain similar expressions for  $\psi_r$ ,  $\psi_l$  and  $\dot{\psi}_r$ . With this notation Eqs. (68) become:

$$\begin{aligned} (\psi_l^1 - i\dot{\psi}_l^1) \circ A_1 + (\psi_l^2 - i\dot{\psi}_l^2) \circ A_2 &= U^{11}(\psi_l^1 + i\dot{\psi}_l^1) \circ A_1 + U^{11}(\psi_l^2 + i\dot{\psi}_l^2) \circ A_2 \\ &\quad + U^{12}(\psi_r^1 + i\dot{\psi}_r^1) \circ A_1 + U^{12}(\psi_r^2 + i\dot{\psi}_r^2) \circ A_2 \end{aligned} \quad (73)$$

$$\begin{aligned} (\psi_r^1 - i\dot{\psi}_r^1) \circ A_1 + (\psi_r^2 - i\dot{\psi}_r^2) \circ A_2 &= U^{21}(\psi_l^1 + i\dot{\psi}_l^1) \circ A_1 + U^{21}(\psi_l^2 + i\dot{\psi}_l^2) \circ A_2 \\ &\quad + U^{22}(\psi_r^1 + i\dot{\psi}_r^1) \circ A_1 + U^{22}(\psi_r^2 + i\dot{\psi}_r^2) \circ A_2 \end{aligned}$$

It will be convenient to use the compact notation  $\psi_{l\pm}^\sigma = \psi_l^\sigma \pm i\dot{\psi}_l^\sigma$ ,  $\sigma = 1, 2$ , and similarly for  $\psi_{r\pm}^\sigma$ .

If  $T$  is a  $n \times n$  matrix and  $X, Y$  arbitrary  $n \times 1$  vectors, we will define  $T \circ X$  as the unique matrix such that  $(T \circ X)Y = T(X \circ Y)$ . The rows of the matrix  $T \circ X$  are  $T_i \circ X$  or alternatively, the columns of  $T \circ X$  are given by  $T^j X_j$  (no summation on  $j$ ). It can be proved easily that

$$T \circ X = T \circ (X \otimes \mathbf{1}), \quad (74)$$

where  $\mathbf{1}$  is the vector whose components are all ones (i.e., the identity with respect to the Hadamard product  $\circ$ ) and the Hadamard product of matrices in the r.h.s. of

Eq. (74) is the trivial componentwise product of matrices. Using these results Eqs. (73) become:

$$(I_n \circ \psi_{l-}^1 - U^{11} \circ \psi_{l+}^1 - U^{12} \circ \psi_{r+}^1)A_1 + (I_n \circ \psi_{r-}^2 - U^{11} \circ \psi_{l+}^2 - U^{12} \circ \psi_{r+}^2)A_2 = 0$$

$$(I_n \circ \psi_{r-}^1 - U^{21} \circ \psi_{l+}^1 - U^{22} \circ \psi_{r+}^1)A_1 + (I_n \circ \psi_{r-}^2 - U^{21} \circ \psi_{l+}^2 - U^{22} \circ \psi_{r+}^2)A_2 = 0$$

Thus the previous equations define a linear system for the  $2n$  unknowns  $A_1$  and  $A_2$ . They will have a non trivial solution if and only if the determinant of the  $2n \times 2n$  matrix of coefficients  $M(U, \lambda)$  below vanish:

$$M(U, \lambda) = \begin{bmatrix} I_n \circ \psi_{l-}^1 - U^{11} \circ \psi_{l+}^1 - U^{12} \circ \psi_{r+}^1 & I_n \circ \psi_{l-}^2 - U^{11} \circ \psi_{l+}^2 - U^{12} \circ \psi_{r+}^2 \\ I_n \circ \psi_{r-}^1 - U^{21} \circ \psi_{l+}^1 - U^{22} \circ \psi_{r+}^1 & I_n \circ \psi_{r-}^2 - U^{21} \circ \psi_{l+}^2 - U^{22} \circ \psi_{r+}^2 \end{bmatrix}.$$

The fundamental matrix  $M(U, \lambda)$  can be written in a more inspiring form using another operation naturally induced by the Hadamard and the usual product of matrices. Thus, consider the  $2n \times 2n$  matrix  $U$  with the block structure of Eq. (69) and the  $2n \times 2$  matrices:

$$[\psi_{\pm}^1 \mid \psi_{\pm}^2] = \left[ \begin{array}{c|c} \psi_{l\pm}^1 & \psi_{l\pm}^2 \\ \hline \psi_{r\pm}^1 & \psi_{r\pm}^2 \end{array} \right],$$

then we define

$$\left[ \begin{array}{c|c} U^{11} & U^{12} \\ \hline U^{21} & U^{22} \end{array} \right] \odot \left[ \begin{array}{c|c} \psi_{l\pm}^1 & \psi_{l\pm}^2 \\ \hline \psi_{r\pm}^1 & \psi_{r\pm}^2 \end{array} \right] \equiv \left[ \begin{array}{c|c} U^{11} \circ \psi_{l\pm}^1 + U^{12} \circ \psi_{r\pm}^1 & U^{11} \circ \psi_{l\pm}^2 + U^{12} \circ \psi_{r\pm}^2 \\ \hline U^{21} \circ \psi_{l\pm}^1 + U^{22} \circ \psi_{r\pm}^1 & U^{21} \circ \psi_{l\pm}^2 + U^{22} \circ \psi_{r\pm}^2 \end{array} \right]$$

and similarly

$$I_{2n} \odot [\psi_{\pm}^1 \mid \psi_{\pm}^2] = \left[ \begin{array}{c|c} I_n \circ \psi_{l\pm}^1 & I_n \circ \psi_{l\pm}^2 \\ \hline I_n \circ \psi_{r\pm}^1 & I_n \circ \psi_{r\pm}^2 \end{array} \right].$$

Finally we conclude that the condition for the existence of coefficients  $A_1$  and  $A_2$  such that the solutions to the eigenvalue equation lie in the domain of the self-adjoint extension defined by  $U$  is given by the vanishing of the spectral function  $\Lambda_U(\lambda) = \det M(U, \lambda)$ , that written with the notation introduced so far becomes:

$$\Lambda_U(\lambda) = \det(I_{2n} \odot [\psi_{-}^1 \mid \psi_{-}^2] - U \odot [\psi_{+}^1 \mid \psi_{+}^2]) = 0. \quad (75)$$

The zeros of the spectral function  $\Lambda$  provide the eigenvalues  $\lambda$  of the spectral problem Eq. (71).

In the particular case  $n = 1$ , the previous equation becomes greatly simplified, the Hadamard product becomes the usual scalar product and the Hadamard-matrix product is the usual product of matrices. After some simple manipulations, the spectral function  $\Lambda_U(\lambda)$  becomes:

$$\Lambda_U(\lambda) = W(l, r, -, -) + U^{11}W(r, l, -, +) + U^{22}W(r, l, +, -) + U^{12}W(r, r, -, +) + U^{21}W(l, l, +, -) + \det U \cdot W(l, r, +, +) \quad (76)$$

where we have used the notation:

$$W(l, l, +, -) = \begin{vmatrix} \psi_{l+}^1 & \psi_{l+}^2 \\ \psi_{l-}^1 & \psi_{l-}^2 \end{vmatrix}, \quad W(l, r, +, -) = \begin{vmatrix} \psi_{l+}^1 & \psi_{l+}^2 \\ \psi_{r-}^1 & \psi_{r-}^2 \end{vmatrix}, \text{ etc.}$$

If we parametrize the unitary matrix  $U \in U(2)$  as:

$$U = e^{i\theta/2} \begin{bmatrix} \alpha & \beta \\ -\bar{\beta} & \bar{\alpha} \end{bmatrix}, \quad |\alpha|^2 + |\beta|^2 = 1,$$

then the spectral function becomes:

$$\Lambda_U(\lambda) = W(l, r, -, -) + \alpha W(r, l, -, +) + \bar{\alpha} W(r, l, +, -) + \beta W(r, r, -, +) - \bar{\beta} W(l, l, +, -) + e^{i\theta} W(l, r, +, +) \quad (77)$$

In particular if we consider a single interval  $[0, 2\pi]$  with trivial Riemannian metric, the fundamental solutions to the equation Eq. (72) have the form  $\Psi^1 = e^{i\sqrt{2\lambda}x}$  and  $\Psi^2 = e^{-i\sqrt{2\lambda}x}$ . Then we have:

$$\begin{aligned} W(l, r, -, -) &= -2i(1 + 2\lambda) \sin(2\pi\sqrt{2\lambda}) - 4\sqrt{2\lambda} \cos(2\pi\sqrt{2\lambda}), \\ W(l, l, +, -) &= 4\sqrt{2\lambda}, \\ W(r, r, -, +) &= 4\sqrt{2\lambda}, \\ W(r, l, -, +) &= 2i(1 - 2\lambda) \sin(2\pi\sqrt{2\lambda}), \\ W(r, l, +, -) &= 2i(1 - 2\lambda) \sin(2\pi\sqrt{2\lambda}), \\ W(l, r, +, +) &= -2i(1 + 2\lambda) \sin(2\pi\sqrt{2\lambda}) + 4\sqrt{2\lambda} \cos(2\pi\sqrt{2\lambda}), \end{aligned}$$

and finally we obtain the spectral function  $\Lambda_U(\lambda)$ :

$$\begin{aligned} \Lambda_U(\lambda) &= -2i(1 + 2\lambda) \sin(2\pi\sqrt{2\lambda}) - 4\sqrt{2\lambda} \cos(2\pi\sqrt{2\lambda}) + 4i \operatorname{Re}(\alpha)(1 - 2\lambda) \sin(2\pi\sqrt{2\lambda}) \\ &\quad + 8 \operatorname{Im}(\beta) \sqrt{2\lambda} + e^{i\theta} [-2i(1 + 2\lambda) \sin(2\pi\sqrt{2\lambda}) + 4\sqrt{2\lambda} \cos(2\pi\sqrt{2\lambda})]. \end{aligned}$$

#### 4.2.3. Quantum wires and quantum Kirchhoff's law

The discussion in the previous section allows to discuss a large variety of self-adjoint extensions of 1D systems whose original configuration space  $\Omega = \sqcup_{\alpha=1}^n [a_\alpha, b_\alpha]$  consist of a disjoint union of closed intervals in  $\mathbb{R}$ . It is clear that some boundary conditions  $U \in U(2n)$  will lead to a quantum system with configuration space a 1D graph whose edges will be the boundary points  $\{a_1, b_1, \dots, a_n, b_n\}$  of the original  $\Omega$  identified among themselves according to  $U$  and with links  $[a_\alpha, b_\alpha]$ .

We will say that the self-adjoint extension determined by a unitary operator  $U$  in  $U(2n)$  defines a quantum wire made of the links  $[a_\alpha, b_\alpha]$  if there exists a permutation  $\sigma$  of  $2n$  elements such that Asorey's condition for  $U$  implies that  $\psi(x_\alpha) = e^{i\beta_\alpha} \psi(x_{\sigma(\alpha)})$ , and  $x_\alpha$  such that  $x_\alpha = a_\alpha$  if  $\alpha = 1, \dots, n$ , or  $x_\alpha = b_{\alpha-n}$  if  $\alpha = n+1, \dots, 2n$ .

Notice that Asorey's condition:

$$\psi - i\dot{\psi} = U(\psi + i\dot{\psi})$$

guarantees that the evolution of the quantum system is unitary, i.e., if we consider for instance a wave packet localized in some interval  $[a_k, b_k]$  at a given time, after a while, the wave packet will have spread out across the edges of the circuit, however

38 *M. Asorey, A. Ibert, G. Marmo*

the probability amplitudes will be preserved. In this sense we may consider Asorey's equation above as the quantum analogue of Kirchhoff's circuit laws, or quantum Kirchhoff's laws for a quantum wire.

## 5. Self-adjoint extensions and semiclassical boundary conditions

### 5.1. Classical boundary conditions and path integrals

The action principle governs the classical and quantum dynamics of unconstrained systems. The classical dynamics is given by stationary trajectories from the variational action principle

$$\left. \frac{\delta S(\mathbf{x}(t))}{\delta \mathbf{x}(t)} \right|_{\mathbf{x}(t)=\mathbf{x}_{cl}(t)} = 0,$$

and the quantum dynamics is automatically implemented in the path integral formalism by the weight that the classical action provides for classical trajectories

$$K_T(x, y) = e^{-TH}(x, y) = \int_{\substack{x(T)=y \\ x(0)=x}} \delta[x(t)] e^{-\frac{1}{2} \int_0^T S(\mathbf{x}(t)) dt}. \quad (78)$$

However, for particles evolving in a bounded domain  $\Omega \subset \mathbb{R}^n$  the variational problem is not uniquely defined. It is necessary to specify the evolution of the particles after reaching the boundary. On the other hand, the very nature of the physical boundary imposes some constraints on the trajectories contributing to the path integral.

In fact, the boundary imposes more severe constraints on the classical dynamics than to the quantum one. This is due to the point-like nature of the particle which requires that after reaching the boundary the individual particle has to emerge back either at the same point or at a different one of the boundary. The only freedom the particle has is where it emerges back and with which momentum it emerges back. The emergence of the particle at a different point covers the possibility that the domain can be folded and glued at the boundary giving rise to non-trivial topologies. In summary, the classical boundary conditions are given by two maps: an isometry of the boundary

$$\alpha : \partial\Omega \rightarrow \partial\Omega$$

and a positive density function

$$\rho : \partial\Omega \rightarrow \mathbb{R}^+$$

which specify the change of position and normal component of momentum of the trajectory of the particle upon reaching the boundary. The isometry  $\alpha$  encodes the possible geometry and topology generated by the folding of the boundary and the function  $\rho$  is associated to the reflectivity (transparency or stickiness) properties of the boundary. Once these two functions are specified the classical variational problem is restricted to trajectories which satisfy the boundary conditions [As04]:

$$\mathbf{x}(t_+) = \alpha(\mathbf{x}(t_-)), \quad (79)$$

$$\boldsymbol{\nu}(\mathbf{x}(t_+)) \cdot \dot{\mathbf{x}}(t_+) = -\rho(\mathbf{x}(t_-)) \boldsymbol{\nu}(\mathbf{x}(t_-)) \cdot \dot{\mathbf{x}}(t_-) \quad (80)$$

40 *M. Asorey, A. Ibort, G. Marmo*

and

$$\begin{aligned} \alpha_*(\dot{\mathbf{x}}(t_-) - [\boldsymbol{\nu}(\mathbf{x}(t_-)) \cdot \dot{\mathbf{x}}(t_-)] \boldsymbol{\nu}(\mathbf{x}(t_-)) \\ = \dot{\mathbf{x}}(t_+) - [\boldsymbol{\nu}(\mathbf{x}(t_+)) \cdot \dot{\mathbf{x}}(t_+)] \boldsymbol{\nu}(\mathbf{x}(t_+)) \end{aligned} \quad (81)$$

for any  $t$  such that  $\mathbf{x}(t) \in \partial\Omega$ , where  $\boldsymbol{\nu}$  denotes the exterior normal derivative at the boundary  $\partial\Omega$  and

$$\mathbf{x}(t_{\pm}) = \lim_{s \rightarrow 0} \mathbf{x}(t \pm s).$$

This definition of classical boundary conditions is motivated by the standard physical heuristic interpretation of boundary conditions. Linear momentum is not conserved because it is partially or totally absorbed by the boundary. The major constraints on the choice of boundary conditions come first by the preservation of the notion of point-like particle which requires that any trajectory which reaches the boundary has to emerge as a single trajectory from the same boundary. The second requirement concerning the permitted changes of linear momentum at the boundary have to be compatible with the action principle. This implies that classical trajectories are determined by the stationary points of the classical action, which for simplicity we assume to be that of a free particle

$$S(\mathbf{x}) = \int dt g_{ij} \dot{x}^i(t) \dot{x}^j(t).$$

The variational principle yields the celebrated Euler-Lagrange motion equations  $\ddot{\mathbf{x}}(t) = 0$  provided that the boundary term

$$\sum_{m=1}^N \left[ \delta\mathbf{x}(t_m^+) \cdot \dot{\mathbf{x}}(t_m^+) - \delta\mathbf{x}(t_m^-) \cdot \dot{\mathbf{x}}(t_m^-) \right] \quad (82)$$

vanishes, where the sum is over all points  $t_m$  where the trajectories reach the boundary. The simpler way of fulfilling this requirement is by imposing the vanishing of each individual term on the sum. These conditions reduce to the boundary conditions (80)(81). provided that the permitted variations are tangent to the boundary. In this case the normal component of  $\delta\mathbf{x}(t_m)$  vanishes, i.e. the points of trajectories which reach the boundary are only allowed to move along the boundary. This condition is reminiscent of Dirichlet condition for D-branes in string theory. The analogue of Neumann boundary conditions is senseless for point-like particles, because it will require to consider only trajectories which reach the boundary with null linear momentum.

Simple but interesting types of boundary conditions already arise in the Sturm-Liouville problem,  $\Omega = [0, 1]$ . In such a case the boundary of the configuration space is a discrete two-points set,  $\partial\Omega = \{0, 1\}$ . Examples of classical boundary conditions in such a case are [As94,As04]:

- i) Neumann (total absorption):  $\alpha = I$ ,  $\rho(0) = \rho(1) = \infty$ .
- ii) Dirichlet (total reflection):  $\alpha = I$ ,  $\rho(0) = \rho(1) = 1$ .



- iii) Periodic:  $\alpha(0) = 1, \alpha(1) = 0, \rho(0) = \rho(1) = 1$ .
- iv) Quasi-periodic:  $\alpha(0) = 1, \alpha(1) = 0, \rho(0) = \rho(1) = \epsilon$ .

All these classical boundary conditions have a quantum counterpart which can be derived from the Feynmann's path integral approach [Fe48,Fe65,Fe50].

### 5.2. Path integrals and quantum boundary conditions

The quantum implementation of classical boundary conditions is straightforward via the path integral method. The only paths to be considered in the Feynman's path integral [Fe48,Fe65,Fe50] given by Eq. (78) are those that satisfy the classical boundary conditions, The corresponding quantum boundary operators are

$$\varphi(\alpha(x)) + i\dot{\varphi}(\alpha(x)) = U [\varphi(\alpha(x)) + i\dot{\varphi}(\alpha(x))] = -\frac{1 - \rho(x) + i}{1 - \rho(x) - i} [\varphi(x) - i\dot{\varphi}(x)].$$

In the one-dimensional case of Sturm-Liouville problem the space of quantum boundary conditions is a four-dimensional Lie group  $U(2)$ , whereas the space of classical boundary conditions is the union of two disconnected two-dimensional manifolds,

$$\mathcal{M}_1 = \{\psi \in L^2([0, 1]), \psi(0) = (1 - \rho_1)\dot{\psi}(1), \psi(1) = (1 - \rho_0)\dot{\psi}(0)\} \quad (83)$$

$$\mathcal{M}_0 = \{\psi \in L^2([0, 1]), \psi(0) = (1 - \rho_0)\dot{\psi}(0), \psi(1) = (1 - \rho_1)\dot{\psi}(1)\} \quad (84)$$

Thus, the Feynman path integral approach does not cover the whole set of boundary conditions. One of the reasons behind the failure of the path integral picture is the single valued nature of trajectories. Many conditions describe a scattering by a singular potential sitting on the boundary. There are two different types of quantum interactions with the boundary: reflection and diffraction. A classical description of the phenomena without including a potential term will require a splitting of the ongoing classical trajectory into two outgoing paths one pointing forward and another one backwards. This picture destroys the pure point-like particle approach and leads to multivalued trajectories which dramatically changes the simple Feynman's description of path integrals. Furthermore, there are boundary conditions where one single trajectory upon reaching the boundary has to be split into an infinite amount of outgoing trajectories. This behaviour can be explicitly pointed out by noticing that the quantum evolution of a narrow wave packet evolves backward after being scattered by boundary as a quite widespread wave packet emerging from all points of the boundary.

In order to have a path integral description of all boundary conditions we need to incorporate some random behaviour for the trajectories reaching the boundary and complex phases for those trajectories. This is possible because the wave functions are complex and the evolution operator involves complex amplitudes. Although in this way we are able to describe any type of unitary evolution in the bounded domain the method goes far beyond Feynman's pure action approach.

The prescription is quite involved and proceeds by considering instead of the Euclidean time evolution propagator  $K_T$  the resolvent operator  $C_z$  of the Hamiltonian

$$C_z(x, y) = (z\mathbb{I} + H)^{-1}(x, y) = \int_0^\infty \frac{dT}{T} e^{-zT} K_T(x, y). \quad (85)$$

The Euclidean time propagator can be recovered from the resolvent by means of the following contour integral

$$K_T(x, y) = \frac{1}{2\pi i} \oint C_z(x, y) e^{zT} dz \quad (86)$$

along a contour which encloses the spectrum of  $H$  on the real axis.

Boundary conditions can be easily implemented into the resolvent, whereas as we shall see, the implementation in the Euclidean time propagator is much harder. Let us consider a fixed boundary condition, e.g. the Neumann boundary conditions  $U_0 = \mathbb{I}$ , and consider the corresponding Hamiltonian  $H_0$  as a background selfadjoint operator. The selfadjoint extension of  $H$  defined on the domain

$$i(\mathbb{I} + U)\dot{\varphi} = (\mathbb{I} - U)\varphi \quad (87)$$

by the unitary operator  $U$  has a resolvent given by Krein's formula [Kr71]

$$C_z^U(x, y) = C_z^0(x, y) - \int_{\partial\Omega} dw \int_{\partial\Omega} dw' C_z^0(x, w) R_z^U(w, w') C_z^0(w', y) \quad (88)$$

where  $R^U$  is the operator of  $L^2(\partial\Omega)$  defined by

$$R_z^U = ((\mathbb{I} - U)C_z^0 - i(I + U))^{-1}(\mathbb{I} - U). \quad (89)$$

A similar formula could be obtained choosing another boundary condition as background boundary condition instead of Neumann's condition.

The inverse transform permits to recover a formula for the propagator kernel of the type

$$K_T(x, y) = K_T^0(x, y) - \frac{1}{2\pi i} \oint dz e^{zT} \int_{\partial\Omega} dw \int_{\partial\Omega} dw' C_z^0(x, w) R_z^U(w, w') C_z^0(w', y). \quad (90)$$

It is easy to rewrite  $K_T^0(x, y)$  as a path integral as in (78) restricting the trajectories to the interior of the domain  $\Omega$  and counting twice the trajectories hitting the boundary  $\partial\Omega$ . However, in general, the kernel  $K_T(x, y)$  cannot be rewritten in terms of a path integral. Only for a few boundary conditions the reduction can be achieved, but for generic boundary conditions the kernel  $K_T(x, y)$  has to be considered as a genuine boundary condition kernel containing information about the boundary jumps amplitudes and phases associated to the different trajectories hitting the boundary. The complex structure of this kernel reduces the utility of the path integral approach and points out the behaviour of the boundary as a genuine quantum device. This behaviour can be explicitly pointed out by noticing that under certain boundary conditions the quantum evolution of a narrow wave

packet is scattered backward by the boundary as a quite widespread wave packet emerging from all points of the boundary. However, there are cases [As07b] where this kernel adopts a simple form and the path integral approach can be formulated in a very explicit way. In particular, for Dirichlet boundary conditions  $U = -\mathbb{I}$ ,

$$R_z^U = (C_z^0)^{-1} \quad (91)$$

and

$$C_z^D(x, y) = C_z^0(x, y) - \int_{\partial\Omega} dw \int_{\partial\Omega} dw' C_z^0(x, w) (C_z^0)^{-1}(w, w') C_z^0(w', y) \quad (92)$$

which leads to a propagator kernel given by the path integral (78) but restricted to paths which do not reach the boundary  $\partial\Omega$ .

The method of images also permits to use unconstrained path integrals to describe systems with non-trivial boundary conditions [Gr93, As07b]. However, in the case of higher dimensions the method is not useful in the presence of non symmetric boundaries and the path integral cannot be defined by a simple prescription as in the Feynman original formulation.

However, the method is only restricted to similar cases and for generic boundary conditions a closed form expression is not available. In higher dimensions the number of boundary conditions for which the path integral method is useful to describe the quantum evolutions is even more limited.

In summary, it is possible to generalise the Feynman approach to describe the dynamics of quantum systems constrained to bounded domains. For some boundary conditions the modification of the path integral formula includes a phase factor or a boundary weight for the trajectories which reach the boundary. However, the method becomes not useful for generic boundary conditions because the prescription becomes very intricate.

## 6. The space of self-adjoint elliptic boundary conditions

### 6.1. *The elliptic Grassmannian*

In the previous sections it was shown that self-adjoint extensions of Dirac and Laplace operators are defined by a family of subspaces (unitary or self-adjoint respect.) of the Hilbert space of boundary data for each operator. However we have not considered whether or not the extensions  $\mathcal{D}_W$  obtained in this way for a Dirac or Laplacian operator  $\mathcal{D}$ , define elliptic operators or not, i.e., if the boundary data given by the subspace  $W$  constitute an elliptic boundary problem for  $\mathcal{D}$ .

This is a crucial point because if the extensions considered were not elliptic, this could affect dramatically the structure of the spectrum (for instance, losing its discreteness), hence affecting the physical properties of the system in unwanted ways. Thus, looking for elliptic extensions of the operator  $\mathcal{D}$  is a way of restricting to a physical sector of the possible theories with ‘good’ spectral properties.

As it was commented in the introduction, the modern theory of elliptic boundary problems for Dirac operators on closed manifolds was developed in the seminal series of papers by Atiyah, Patodi and Singer [At68] and, on manifolds with boundary, [At75]. The boundary conditions introduced there to study the index theorem for Dirac operators on even-dimensional spin manifolds with boundary are nowadays called Atiyah-Patodi-Singer boundary conditions (APS BC’s). The crucial observation there was that global boundary conditions were needed in order to obtain an elliptic problem, contrary to the situation for second order operators where (local) Dirichlet conditions, for instance, are elliptic. Such boundary conditions were extended to include also odd dimensional spin manifolds with boundary (see [Da94] and references therein).

Later on, E. Witten ([Wi88], §II), pointed out the link between elliptic boundary conditions for the Dirac operator on 2 dimensions and the infinite dimensional Grassmannian manifold. The infinite dimensional Grassmannian was introduced previously in the analysis of integrable hierarchies and discussed extensively by Segal and Wilson (see [Se85] and references therein). More recently Schwarz and Friedlander [Fr97] have extended Witten’s analysis to arbitrary elliptic operators on arbitrary dimensional manifolds with boundary. The particular analysis for Dirac operators we are using follows from [At75] but it can be extended also to higher order operators. More comments on this will be found later on.

The basic idea is that the space of zero modes of a Dirac (or Laplace) operator  $\mathcal{D}$ ,  $\ker \mathcal{D} = \{ \xi \in \Gamma(S) \mid \mathcal{D}\xi = 0 \}$ , induces a subspace at the boundary  $b(\ker \mathcal{D})$  that in general will be infinite-dimensional, hence a way to restore ellipticity will be to restrict to a subspace such that the kernel and cokernel of the operator defined on this subspace will be finite dimensional. We will perform such analysis for the Dirac and Laplace operators and we will refer to [Fr97] for the general case.

The analysis of such projection requires a detailed description of solutions near the boundary. Assuming that the Riemannian metric on  $\Omega$  is a product near the boundary  $\partial\Omega$ , we can decompose the operator  $\mathcal{D}$  in a collar neighborhood  $U_\epsilon(-\epsilon, 0] \times$

$\partial\Omega$  of the boundary as (Eq. (39)):

$$\not{D} = \nu \cdot (\partial_\nu + \not{D}_{\partial\Omega}),$$

where  $\not{D}_{\partial\Omega}$  is the Dirac operator on the boundary bundle  $S_{\partial\Omega}$ . A natural set of boundary conditions for our problem will be constructed as follows.

Recall from §3.4 that  $\not{D}_{\partial\Omega}$  is an elliptic and, because  $\partial\Omega$  is closed, essentially self-adjoint differential operator on  $\partial\Omega$  that anticommutes with  $J$ , i.e.  $\not{D}_{\partial\Omega}J = -J\not{D}_{\partial\Omega}$ . The Dirac Laplacian  $\not{D}_{\partial\Omega}^2$  is a non-negative self-adjoint elliptic operator with a real discrete spectrum  $\text{Spec } \not{D}_{\partial\Omega}^2 = \{\mu_k \mid 0 \leq \mu_0 < \mu_1 < \dots\}$  and such that the eigenspaces  $E(\lambda_k)$  are finite dimensional,  $E(\mu_k) = \{\phi_k \in \mathcal{H}_D \mid \not{D}_{\partial\Omega}^2 \phi_k = \mu_k \phi_k\}$ . The kernel  $K$  of  $\not{D}_{\partial\Omega}$  agrees with  $\ker \not{D}_{\partial\Omega}^2$  and with  $E(0)$ . We have thus the following orthogonal decomposition of  $\mathcal{H}_D$ ,

$$\mathcal{H}_D = \bigoplus_{k=0}^{\infty} E(\mu_k) = K \oplus \bigoplus_{k=1}^{\infty} (E_+(\lambda_k) \oplus E_-(\lambda_k)),$$

where we have set  $E(\mu_k) = E_+(\lambda_k) \oplus E_-(\lambda_k)$ , with  $\lambda_{\pm k} = \pm\sqrt{\mu_k}$ . Then the spectrum of  $\not{D}_{\partial\Omega}$  is given by  $\{\pm\lambda_k\}$ . Moreover if we denote by  $\text{Spec}_+$  the non-negative spectrum of  $\not{D}$ , and by  $\text{Spec}_-$  its negative spectrum, then we may write

$$\mathcal{H}_D = \bigoplus_{\lambda \in \text{Spec}_+} E_+(\lambda) \oplus \bigoplus_{\lambda \in \text{Spec}_-} E_-(\lambda).$$

The subspaces  $T_+ = \bigoplus_{\lambda \in \text{Spec}_+} E_+(\lambda)$  and  $T_- = \bigoplus_{\lambda \in \text{Spec}_-} E_-(\lambda)$  define a polarisation of  $\mathcal{H}_D$ . Denoting by  $P_{\pm} \mathcal{H} \rightarrow T_{\pm}$  the corresponding orthogonal projectors, the celebrated Atiyah-Patodi-Singer boundary conditions (APS BC) are given by the (non-local) condition:

$$P_+ b(\xi) = 0, \quad \xi \in H^1(\Omega, S).$$

In other words, APS BC select the negative spectrum of the boundary Dirac's operator  $\not{D}_{\partial\Omega}$ .

On the other hand the polarization  $\mathcal{H}_D = \mathcal{H}_+ \oplus \mathcal{H}_-$  defined by the compatible complex structure  $J_D$ ,  $J_D(\mathcal{H}_{\pm}) = \mp i\mathcal{H}_{\pm}$ , induces a decomposition of the eigenspaces  $E(\lambda_k)$  as

$$E(\lambda_k) = E_{\pm}(\lambda_k) = E(\lambda_k) \cap \mathcal{H}_{\pm}.$$

Moreover,  $\not{D}_{\partial\Omega}$  restricts to a map  $\not{D}_k = \not{D}_{\partial\Omega}|_{E(\lambda_k)}: E(\lambda_k) \rightarrow E(\lambda_k)$  and because it anticommutes with  $J$ , we have that  $\not{D}_k: E_{\pm}(\lambda_k) \rightarrow E_{\mp}(\lambda_k)$ , thus  $\not{D}_k$  has the following block structure,

$$\not{D}_k = \left( \begin{array}{c|c} 0 & \not{D}_k^+ \\ \hline \not{D}_k^- & 0 \end{array} \right),$$

and because  $\not{D}_k$  is self-adjoint,  $(\not{D}_k^-)^{\dagger} = \not{D}_k^+$ . On the other hand  $\not{D}_k^2 = \not{D}_{\partial\Omega}^2|_{E(\lambda_k)} = \lambda_k I$ , hence the spectrum of  $\not{D}_k$  on  $E(\lambda_k)$  consists of  $\pm\sqrt{\lambda_k}$ . The operator  $\not{D}_k$  is invertible in  $E(\lambda_k)$  for  $k \geq 1$ , hence  $\dim E_+(\lambda_k) = \dim E_-(\lambda_k)$ . Moreover  $K =$

$K_+ \oplus K_-$ , and  $\dim K_+ = \dim K_-$ . In fact the index of the operator  $\mathcal{D}_0^+$  is zero because  $\partial\Omega$  is cobordant to  $\emptyset$  and the index is cobordant invariant. We can choose an orthonormal basis  $\phi_{k,\alpha}^\pm \in E_\pm(\lambda_k)$ ,  $\alpha = 1, \dots, \dim E_\pm(\lambda_k)$ , such that

$$\mathcal{D}_k \phi_{k,\alpha}^\pm = \pm i \sqrt{\lambda_k} \phi_{k,\alpha}^\mp.$$

The Cayley transform discussed in §2.3 diagonalizes the operators  $\mathcal{D}_k$ , and we have

$$\xi_{k,\alpha}^\pm = \phi_{k,\alpha}^+ \pm i \phi_{k,\alpha}^- \in \mathcal{L}_\pm,$$

and

$$\mathcal{D}_k \xi_{k,\alpha}^\pm = \pm \sqrt{\lambda_k} \xi_{k,\alpha}^\pm.$$

Then, it is clear that  $b(\ker \mathcal{D}_{\text{APS}}) = \mathcal{L}_+$ . Moreover the orthogonal projectors  $\text{pr}_\pm: \mathcal{H}_D \rightarrow \mathcal{L}_\pm$  are pseudodifferential operators whose complete symbol depends only on the coefficients of  $\mathcal{D}$ . Thus, elliptic boundary conditions will be defined by subspaces  $W \subset \mathcal{H}_D$  such that  $W \cap \mathcal{L}_+$  will be finite dimensional (notice that such intersection corresponds to solutions of  $\mathcal{D}\xi = 0$  with boundary values on  $W$ ), this means that the projection  $\text{pr}_+|_W$  will have a finite dimensional kernel. Moreover, the cokernel of  $\text{pr}_+$  will have to be finite-dimensional if  $\mathcal{D}^\dagger$  is elliptic too. Finally, if the extension  $\mathcal{D}_W$  is elliptic, then there will exist left and right parametrices for it, and this will imply that the projection  $\text{pr}_-|_W$  will have to be compact operators. It is sometimes convenient to restrict the last assumption to operators of Hilbert-Schmidt class. We can conclude that the set of closed subspaces  $W$  of  $\mathcal{H}_D$  verifying the following conditions:

- i.  $\text{pr}_+|_W: W \rightarrow \mathcal{L}_+$  is Fredholm.
- ii.  $\text{pr}_-|_W: W \rightarrow \mathcal{L}_-$  is Hilbert-Schmidt,

determines all elliptic extensions of the Dirac operator  $\mathcal{D}$ . Such space will be called the elliptic infinite dimensional Grassmannian of  $\mathcal{D}$ , or elliptic Grassmannian for short and will be denoted by  $\text{Gr}(\mathcal{L}_-, \mathcal{L}_+)$ .

The elliptic Grassmannian can be constructed also in terms of the polarization  $\mathcal{H}_+ \oplus \mathcal{H}_-$  instead of  $\mathcal{L}_+ \oplus \mathcal{L}_-$ . This is the approach taken for instance in [Da94]. In such case, we will relate self-adjoint extensions of  $\mathcal{D}$  with unitary operators  $U: \mathcal{H}_+ \rightarrow \mathcal{H}_-$ , hence elliptic boundary conditions correspond to unitary operators  $U$  such that the projection from its graph to  $\mathcal{H}_+$  would be Fredholm and the projection onto  $\mathcal{H}_-$  would be Hilbert-Schmidt. It is obvious that the Cayley transform  $C$  defines a one-to-one map from  $\text{Gr}(\mathcal{H}_-, \mathcal{H}_+)$  into  $\text{Gr}(\mathcal{L}_-, \mathcal{L}_+)$  (the map is actually a diffeomorphism, see below), but it is important to keep in mind that the objects in the two realizations of the Grassmannian are different.

We will call in what follows the elliptic boundary conditions defined by points in the elliptic Grassmannian, generalized APS boundary conditions. It is important to point it out here that a parallel discussion takes place for the discussion of elliptic extensions of the Laplacian operator. In fact replacing  $\mathcal{H}_D$  by  $\mathcal{H}_B$ ,  $J_D$

by  $J_B$  and considering the boundary Laplacian  $-\Delta_{\partial\Omega}$  we will obtain that the elliptic extensions of  $-\Delta$  are in one-to-one correspondence with points in the elliptic Grassmannian  $\text{Gr}(\mathcal{L}_-, \mathcal{L}_+)$ , and similarly, by using the Cayley transform, with points in the elliptic Grassmannian  $\text{Gr}(\mathcal{H}_-, \mathcal{H}_+)$ . Hence, in what follows we will omit the subindex in the notation of the different boundary Hilbert spaces and operators and we will refer simultaneously to the Dirac and/or Laplacian operators, and the elliptic Grassmannian defining their elliptic extensions will be denoted simply by  $\mathbf{Gr}$ .

The elliptic infinite dimensional Grassmannian has an important geometrical and topological structure. We must recall first (see for instance Pressley and Segal [Pr86] for more details) that  $\mathbf{Gr}$  is a smooth manifold whose tangent space at the point  $W$  is given by the Hilbert space of Hilbert-Schmidt operators  $\mathcal{J}_2(\mathcal{L}_-, \mathcal{L}_+)$ , from  $\mathcal{L}_-$  to  $\mathcal{L}_+$ . The group of linear continuous invertible operators  $GL(\mathcal{H})$  does not act on  $\mathbf{Gr}$  but only a subgroup of it, the restricted general linear group  $GL_{\text{res}}(\mathcal{H})$ , which defines the restricted unitary group  $U_{\text{res}}(\mathcal{H}) = GL_{\text{res}}(\mathcal{H}) \cap U(\mathcal{H})$ . The groups  $GL(\mathcal{H})$  and  $U(\mathcal{H})$  are contractible but  $GL_{\text{res}}(\mathcal{H})$  and  $U_{\text{res}}(\mathcal{H})$  are not. The manifold  $\mathbf{Gr}$  is not connected and is decomposed in its connected components defined by the virtual dimension of their points which is simply the index of the Fredholm operator  $pr_+|_W$ , then,  $\mathbf{Gr} = \cup_{k \in \mathbb{Z}} \text{Gr}^{(k)}$ .

The Grassmannian  $\text{Gr}(\mathcal{L}_-, \mathcal{L}_+)$  carries a natural Kähler structure defined by the hermitian structure given by

$$h_W(\dot{A}, \dot{B}) = \text{Tr } \dot{A}^\dagger \dot{B},$$

where  $\dot{A}, \dot{B} \in T_W \text{Gr}(\mathcal{L}_-, \mathcal{L}_+)$  are Hilbert-Schmidt operators from  $\mathcal{L}_-$  to  $\mathcal{L}_+$ . The imaginary part defines a canonical symplectic structure  $\omega$ ,

$$\omega_W(\dot{A}, \dot{B}) = -\frac{i}{2} \text{Tr } (\dot{A}^\dagger \dot{B} - \dot{B}^\dagger \dot{A}). \quad (93)$$

The elliptic Grassmannian is quasicompact in the sense that the only holomorphic functions are constant.

## 6.2. The space of self-adjoint extensions: the self-adjoint Grassmannian and elliptic self-adjoint extensions

We have characterized the self-adjoint extensions of a given Dirac or Laplacian operators as the space  $\mathcal{M}$  of self-adjoint subspaces of a boundary Hilbert space  $\mathcal{H}$  carrying a polarization  $\mathcal{H} = \mathcal{L}_- \oplus \mathcal{L}_+$ . On the other hand, we have seen in the previous section that the Grassmannian  $\text{Gr}(\mathcal{L}_-, \mathcal{L}_+)$  describes the elliptic extensions of such operator. Then, the elliptic self-adjoint extensions of the given operators will be given by the intersection  $\mathcal{M} \cap \text{Gr}(\mathcal{L}_-, \mathcal{L}_+)$ . This space will be called the elliptic self-adjoint Grassmannian or the self-adjoint Grassmannian for short. It is possible to see that the self-adjoint Grassmannian is a smooth submanifold of the Grassmannian and decomposes in connected components which are submanifolds of the components  $\text{Gr}^{(k)}$ . We will denote the elliptic self-adjoint Grassmannian

as  $\mathcal{M}_{\text{ellip}}$ . The most relevant topological and geometrical aspects of  $\mathcal{M}_{\text{ellip}}$  are contained in the following theorem.

**Theorem 11.** *The elliptic self-adjoint Grassmannian  $\mathcal{M}_{\text{ellip}}$  is a Lagrangian submanifold of the infinite dimensional Grassmannian  $\mathbf{Gr}$ .*

**Proof.** That  $\mathcal{M}_{\text{ellip}}$  is an isotropic submanifold of  $\text{Gr}(\mathcal{L}_-, \mathcal{L}_+)$  follows immediately from Eq. (93) and the observation that tangent vectors to  $\mathcal{M}_{\text{ellip}}$  at  $W$  are defined by self-adjoint operators.

Now, all we have to do is to compute  $T_W \mathcal{M}_{\text{ellip}}^\perp$  at  $W = 0$  because of the homogeneity of the Grassmannian. Hence, if  $\dot{A} \in T_0 \mathcal{M}_{\text{ellip}}^\perp$ , this means that

$$\text{Tr}(\dot{A}^\dagger \dot{B} - \dot{B} \dot{A}) = 0,$$

for every self-adjoint  $\dot{B} \in \mathcal{J}_2(\mathcal{L}_-, \mathcal{L}_+)$ , hence  $\dot{A}^\dagger - \dot{A} = 0$ , and  $\dot{A}$  is self-adjoint, then lying in  $T\mathcal{M}_{\text{ellip}}$ .  $\square$

A Lagrangian submanifold of a compact manifold carries a characteristic class called the Maslov class which is an element of first cohomology group of the manifold with integer coefficients. The Maslov class is the dual of the Maslov cycle as constructed by Arnold [Ar67]. For reasons that will be clear later on we will call the dual of the Maslov class for  $\mathcal{M}_{\text{ellip}}$  the Cayley-Maslov surface and we will devote the remaining part of this section to describe this cycle and the Maslov class of  $\mathcal{M}_{\text{ellip}}$ ,  $\nu \in H^1(\mathcal{M}_{\text{ellip}}, \mathbb{Z})$ .

The Cayley-Maslov surface  $\mathcal{C}$  is the subspace of the self-adjoint Grassmannian  $\mathcal{M}_{\text{ellip}}$  that contains the self-adjoint subspaces that cut  $L_-$  in a space of dimension  $\geq 1$ . The Cayley-Maslov subspace  $\mathcal{C}$ , is a stratified manifold,  $\mathcal{C} = \cup_{k \geq 1} \mathcal{C}^{(k)}$ , that contains an open dense submanifold consisting of the space of self-adjoint subspaces whose intersection with  $\mathcal{L}_-$  is exactly 1, the space denoted by  $\mathcal{C}^{(1)}$ . This is enough for topological purposes to analyze the crossings of the Cayley-Maslov surface. In what follows we will denote  $\mathcal{C}^{(1)}$  simply by  $\mathcal{C}$  and we will call it the Cayley-Maslov surface. In [Ar67] it is proved that the Cayley-Maslov surface is two sided. The proof works exactly the same in our setting, i.e., there is a non-vanishing vector field transversal to it and given by the tangent vector to the curve of self-adjoint operators,

$$A_t = \frac{A - \tan \frac{tI}{2}}{\tan \frac{tA}{2} + I},$$

which is simply the image by the Cayley transform of the curve in the space of unitary operators obtained by multiplication by  $\exp it$ . We will call the positive side of the Cayley surface the exiting of the previous curve and the negative side the exiting of the curve  $A_{-t}$ .

Given a continuous curve  $\gamma: [0, 1] \rightarrow \mathcal{M}_{\text{ellip}}$  we will define its index as the sum of positive crossing minus the sum of negative crossings, where a crossing is positive if



it is done from the negative to the positive side and negative conversely. For curves in general position such number will be finite.

The Cayley-Maslov surface defined in this way can be called the Cayley-Maslov cycle of the self-adjoint Grassmannian and the Cayley index is simply the intersection index of the Cayley cycle. The identification of the self-adjoint Grassmannian with a subgroup of unitary operators allows for an alternative cohomological way of computing such index.

We should remark first that if  $W_A$  is a generic element in the self-adjoint Grassmannian, the corresponding unitary operator  $U_A$  given by its Cayley transform is of the form  $I + K_A$  where  $K_A$  is Hilbert-Schmidt. In fact, it is clear that

$$K_A = \frac{2iA}{I - iA},$$

hence,

$$K_A^\dagger K_A = \frac{4A^2}{I + A^2},$$

and then,

$$\text{Tr } K_A^\dagger K_A = 4 \text{Tr } \frac{A^2}{I + A^2} \leq 4 \text{Tr } A^2 < \infty.$$

Then, we can define the determinant of  $U_A$  in an standard way using the regularized determinant

$$\lg \det' U = \sum_{i=1}^{\infty} \lg \frac{1 + k_i}{e^{k_i}},$$

which is finite for all unitary operators differing from the unity by a Hilbert-Schmidt operator.

Given a closed curve  $\gamma: S^1 \rightarrow U(\mathcal{H}_+, \mathcal{H}_-)$  whose image lies in the image by the Cayley transform of the self-adjoint Grassmannian, i.e.  $\gamma \in C(\mathcal{M}_{\text{ellip}})$ , we will define the index of  $\gamma$  as the winding number of the curve  $\det' \circ \gamma: S^1 \rightarrow S^1$ , in other words,

$$\sharp(\gamma) = \frac{1}{2\pi} \int_0^{2\pi} \det'(\gamma(\theta)) d\theta = \frac{1}{2\pi} \int_{S^1} (\det')^* d\theta.$$

In order to show that the winding number  $\sharp\gamma$  coincides with the Cayley index of  $\gamma$  we are going to introduce an alternative way of computing such winding number.

Given a unitary operator we will define its degenerate dimension as the dimension of the eigenspace with eigenvalue 1. If  $U$  is of the form above,  $U = I + K$  with  $K$  Hilbert-Schmidt, then the dimension of the eigenspace of eigenvalue 1 is finite and the degenerate dimension of the operator is finite. We shall denote such number by  $\nu(U)$ . If  $U_t$  is a curve  $\gamma$  of such unitary operators, then we define the index of such curve as

$$\nu(\gamma) = \int_0^1 \nu(U_t) dt. \quad (94)$$

We can see that  $\nu(U_t)$  is of bounded variation because of the continuity on the norm topology on the space  $C(\mathcal{M}_{\text{ellip}})$ , then the integral in Eq. (94) is finite.

**Theorem 12.**  $\sharp\gamma = \nu(\gamma)$ .

**Proof.** The crucial observation to prove the formula above is to realize that  $\nu(\gamma)$  is the net number of eigenvalues of  $U_t$  that cross through  $-1$ . On the other hand after subtracting a global term in the definition of the determinant  $\det' U_t$  which corresponds to the eigenvalues that do not move away of a compact set, the others, a finite number, wind around the unit circle, and the determinant counts the sum of the winding number of all of them. Then, the equality follows.  $\square$

The previous index will be called the Cayley-Maslov class and it defines a non-trivial cohomology class in  $H^1(\mathcal{M}_{\text{ellip}}, \mathbb{Z})$ .

**Theorem 13.** *The Cayley index of a curve  $\gamma$  and the winding number  $\sharp\gamma$  of  $\gamma$  agree.*

This follows easily from the fact that crossing the eigenvalue  $-1$  for a curve  $U_t$  of unitary operators is equivalent to  $A_{U_t}$  crossing the Cayley surface in  $\Lambda_S$ . Thus counting the crossings in both pictures gives the same number.

If we perform an adiabatic change in the boundary conditions defining self-adjoint extensions of the operator  $\mathbb{H}$ , the spectrum of such extensions will change. It could happen that in such deformation process we will approach an unstable sector of the theory. This will happen when crossing the Cayley surface. On the other hand, as it was discussed before, the number of crossings of the Cayley surface with appropriate signs defines an integer number that is related to the topology of the space of elliptic self-adjoint extensions. We will call it the Cayley index and it has a similar geometrical origin as the Maslov-Arnold index but quite a different physical meaning.

## 7. Self-adjoint extensions of dissipative systems

In discussing self-adjoint extensions of symmetric elliptic operators we have found that they are described by a Lagrangian submanifold in the universal infinite dimensional elliptic Grassmannian. The remaining describes extensions that are not self-adjoint. We will start in this section a discussion on the meaning of such extensions, both mathematically and physically. From this discussion we will learn that the self-adjointness of these extensions can be restored adding an external “effective” Hilbert space to our system.

### 7.1. Non-self-adjoint extensions and local evolution

To set up the discussion in concrete terms we will consider a particle moving freely on a Riemannian manifold  $(\Omega, \eta)$  with boundary  $\partial\Omega \neq \emptyset$ , and described in quantum mechanical terms by the Laplace-Beltrami Hamiltonian  $H_0 = -\frac{1}{2}\Delta$ .

Let  $W$  be a non-selfadjoint subspace of the elliptic Grassmannian  $\mathbf{Gr}$ , i.e.,  $W \neq W^\dagger$ . If  $W$  is the graph of an operator  $T$ , this means that  $T$  is non-selfadjoint. Moreover the Cayley transform on  $T$  will define a linear isomorphism  $C_T: \mathcal{H}_+ \rightarrow \mathcal{H}_-$  that will not be unitary.

This lack of unitarity reflects the fact that probability is not preserved at the boundary, i.e., the non-unitary evolution semigroup defined by the extended operator will not preserve the norm of states and, for instance, states could “evaporate”.

Another way of putting it is that this situation is describing a dissipation of some type acting on the system. Because of the structure of the system (the operator is symmetric on the interior of  $\Omega$ ) the only place where this dissipation can occur is at the boundary, however localized as it is, it affects instantaneously the system as a whole. We may discuss this aspect briefly.

It is well known that a free non-relativistic wave packet localized in a bounded region at time  $t = 0$  spreads instantaneously over all of space [He98]. Thus if we consider a quantum system defined on a manifold with boundary with self-adjoint boundary conditions, and we modify them to non-self-adjoint ones, i.e., the system becomes dissipative, such modification, even if it is performed adiabatically, will affect the state of the system instantaneously even if such state is localized far away from the boundary contrary to what a naive perturbative analysis would suggest.

To make this analysis more precise, let us consider a fixed smooth section  $\Psi_0$  with compact support  $K = \text{supp}\Psi$  on the interior of  $\Omega$ , that is  $\Psi \in C_0^\infty(\Omega)$ . Then we may consider a larger open set  $\mathcal{U} \subset \overline{\mathcal{U}} \subset \Omega \cup \partial\Omega$ . Then consider the smooth manifold  $\Omega' = \overline{\mathcal{U}}$  with boundary  $\partial\Omega' = \overline{\mathcal{U}} - \mathcal{U}$ . If we denote by  $\iota: \Omega' \rightarrow \Omega$  the canonical embedding, then we equip  $\Omega'$  with the Riemannian metric  $\iota^*\eta$  that we will denote  $\eta'$ . In the same way we may pull-back to  $\Omega'$  any further structure on  $\Omega$ , a vector bundle  $E \rightarrow \Omega$ , a connection  $\nabla: \Gamma(E) \rightarrow \Gamma(E \otimes T^*\Omega)$ , etc., that will be denoted in the same fashion  $E'$ ,  $\nabla'$ , etc. Now we may consider the Hilbert space  $L^2(\Omega', E')$  of square integrable sections of the pull-back of the bundle  $E$  over  $\Omega$  to  $\Omega'$  with

respect to the metric  $\eta'$ . The Laplace-Beltrami operator on  $\Omega'$  defines a symmetric operator on  $L^2(\Omega', E')$  and Dirichlet's boundary conditions provide a self-adjoint extension of it.

There is a natural continuous isometry from  $L^2(\Omega', E')$  to  $L^2(\Omega, E)$ , induced by the embedding map  $\iota_*: C_c^\infty(E') \rightarrow C_c^\infty(E)$  given by  $(\iota_*\Psi)(x) = \Psi(x')$ , if  $x = \iota(x')$ ,  $x' \in \Omega'$ , and 0 otherwise. Notice that:

$$\|\iota_*\Psi\|_{L^2(\Omega, E)}^2 = \int_{\Omega} |\Psi(x)|^2 \text{vol}_{\eta} = \int_{\Omega'} |\Psi(x')|^2 \text{vol}_{\eta'} = \|\Psi\|_{L^2(\Omega', E')}^2 \quad \forall \Psi \in C_c^\infty(E'),$$

hence, because both spaces  $C_c^\infty(E')$  and  $C_c^\infty(E)$  are dense in  $L^2(\Omega', E')$  and  $L^2(\Omega, E)$  respectively,  $\iota_*$  extends to an isometry  $\hat{\iota}: L^2(\Omega', E') \rightarrow L^2(\Omega, E)$ . In this sense we may consider  $L^2(\Omega', E')$  as a closed subspace of  $L^2(\Omega, E)$ . Notice now that  $\Psi_0 \in L^2(\Omega', E')$  by construction.

Let  $H_W$  be the elliptic extension of the Laplace-Beltrami operator determined by the boundary conditions defined by the subspace  $W$ . Because of the correspondence between elliptic boundary conditions and subspaces  $N$  of the deficiency space  $\mathcal{N}$  of the operator  $H_0$ , then the extension of the operator defined by the subspace  $N$  has a domain  $D_W = D_0 \oplus N$ , and it acts on an state  $\Psi = \Psi_0 + \xi$ ,  $\Psi_0 \in D_0, \xi \in N$ , as  $H_W(\Psi) = H_0\Psi_0 + K\xi$ . But in the situation above the state  $\Psi_0$  that we will use as initial data for the evolution problem:

$$i\frac{\partial}{\partial t}\Psi = H_W\Psi, \quad \Psi \in D_K, \quad (95)$$

lies in  $D_0$ , the minimal extension domain, hence:

$$H_W\Psi_0 = H_0\Psi_0 = H_D\Psi_0,$$

where  $H_D$  is the minimal selfadjoint extension corresponding to Dirichlet boundary conditions  $\Psi \in D_D(\Omega'), \Psi|_{\partial\Omega'} = 0$ .

However, one can show that even if any power  $n$  of the Hamiltonian satisfies:

$$H_W^n\Psi_0 = H_D^n\Psi_0,$$

the actual evolutions of the system governed by  $H_W$  is very different from that governed by Dirichlet boundary conditions. This different behaviour is due to the fact that the local time evolution of the quantum system is not perturbative in  $t$ .

In fact, that is exactly what from a physical perspective we should expect; the system under study is in contact with an exterior system represented by the boundary. The interaction between them is represented by an “effective” action described by the boundary conditions and they contribute instantaneously to the evolution of the system.

For instance we can imagine that the boundary is an actual boundary made of a semitransparent mirror or membrane, with a given coefficient of reflection and transmission. Then, a given fraction of the probability amplitude will be transmitted to the exterior part of the membrane and the evolution from the point of view of the system inside the membrane will not be unitary. This kind of situations have

been studied in a variety of situations (see for instance a detailed discussion of this type of boundary conditions for interfaces of two quantum systems by Popov [Po95] and references therein).

### 7.2. Unitarization of non-self-adjoint boundary conditions

Thus, dissipation at the boundary from the previous viewpoint will be modeled by a non-unitary isomorphism  $F$  at the boundary. Such isomorphism will replace the exterior system that is in contact with the inner one.

It is important to observe that the full system, the initial or interior system plus the exterior system, being closed has to be described by unitary evolution. In this sense the non-unitarity of the evolution of the system under the boundary condition  $F$  is restored adding an external system that takes into account the dissipation at the boundary.

Thus, given a dissipative quantum system  $H$  described by a non-selfadjoint extension  $F$ , the idea to restore its unitarity (within a larger system, of course) will be to construct an enlarged unitary quantum system such that our system will be a (non-unitary) subsystem. A natural requirement to ask to this enlarged quantum system is to be as small as possible, that is minimal in the class of such enlargements, i.e., the smallest possible unitary quantum system in which we can embed the non-unitary one. We will call such enlargement an unitarization of the dissipative system  $(H, F)$ .

At the classical level this idea can be implemented easily by using symplectic geometry. Different approaches can be taken that will eventually lead to the construction of adequate quantum models. We will only sketch them here, leaving a detailed discussion of them and their quantum counterparts to further work.

Let  $M$  be a symplectic manifold with symplectic form  $\omega$ , for instance  $M$  could be the cotangent bundle  $T^*\Omega$  of a mechanical system with configuration space  $\Omega$ . Let us consider now a vector field  $X$  on  $M$  representing the dynamical evolution of a classical physical system which is not necessarily Hamiltonian, i.e., such that  $\mathcal{L}_X\omega \neq 0$ . Let  $\alpha_X$  denote the exact 2-form such that  $\alpha_X = \mathcal{L}_X\omega$ ,  $\alpha_X = d(i_X\omega)$ .

If we solve now the equation

$$\mathcal{L}_X\beta = \alpha_X, \quad (96)$$

with the requirement that  $\beta$  is a closed 2-form with maximal dimensional kernel (notice that  $\omega$  is a solution with minimal dimensional kernel), we can redefine the structure form  $\omega$  as

$$\sigma = \omega - \beta,$$

and obviously,  $\mathcal{L}_X\sigma = 0$ .

Now our vector field  $X$  is a Hamiltonian vector field for the closed 2-form  $\sigma$  (which is non-unique), however the form  $\sigma$  can fail to be symplectic because its rank can be strictly lower than that of  $\omega$ , i.e.,  $\sigma$  will define a presymplectic structure on

$M$ . We must point it out that the eq. (96) has always a solution which is  $\omega$  itself, but if it were the only one, then the 2-form  $\sigma = 0$ .

The triple  $(M, \sigma, X)$  can be naturally extended to a Hamiltonian system using the well-known coisotropic embedding theorem [Go81], that states that there is a symplectic manifold  $(P, \tilde{\sigma})$  and a Hamiltonian vector field  $\tilde{X}$  on it such that there is a canonical embedding  $j: M \rightarrow P$  such that  $j^*\tilde{\sigma} = \sigma$ ,  $\tilde{X}$  is tangent to the submanifold  $j(M) \subset P$  and  $\tilde{X}|_{j(M)} = j_*X$ .

The total space  $P$  is a tubular neighborhood of the zero section of the bundle  $\ker \sigma^* \rightarrow M$ , where  $\ker \sigma^*$  is the dual of the subbundle  $\ker \sigma \subset TM$ . The vector field  $X$  induces a function on  $P$  as follows

$$P_X(x, \zeta) = \langle \zeta(x), X(x) \rangle, \quad \forall x \in M, \quad \zeta \in \ker \omega^*,$$

and the corresponding Hamiltonian vector field  $\tilde{X}$  on  $P$  restricts to  $X$  on the submanifold  $M$ . In this picture the minimal extension is obtained by “adding” the dual of the kernel of  $\sigma$  to our original space. Notice again that if Eq. (96) had only one solution  $\beta = \omega$ , then  $\sigma = 0$  and  $P = T^*M$ . The Hamiltonian vector field  $\tilde{X}$  becomes the complete lift  $X^c$  of  $X$  to  $T^*M$ .

There is an alternative way to present the previous discussion. It consists in considering again a vector field  $X$  which is not Hamiltonian. This vector field will represent the non-unitary evolution semigroup at the quantum level. The graph of the vector field defines a submanifold, denoted again by  $X$ , of  $TM$ .

If the vector field were Hamiltonian, the submanifold  $X$  would be Lagrangian with respect to the natural symplectic form  $\hat{\omega}$  in  $TM$ . In general we will obtain that  $TX \neq TX^\perp$ , where  $\perp$  means the symplectic orthogonal with respect to  $\omega$ . The distribution on  $X$  defined by  $TX \cap TX^\perp$  (provided that the intersection is clean) is integrable as it is easily seen by computing  $\omega([U, V], Z)$  for  $U, V \in TX \cap TX^\perp$  and  $Z \in TX$ .

Then the quotient  $TX/TX \cap TX^\perp$  is a symplectic bundle. Denoting by  $\mathcal{F}$  the foliation defined by  $TX \cap TX^\perp$ , if the space of leaves  $\mathcal{S}_X = X/\mathcal{F}$  of this foliation is a manifold, then  $TX/TX \cap TX^\perp$  can be identified with its tangent bundle  $T(X/\mathcal{F})$ . Then, the induced form from  $\hat{\omega}$  on  $TX/TX \cap TX^\perp$  will define a non-degenerate, closed, smooth 2-form on  $\mathcal{S}_X$  making in this way  $\mathcal{S}_X$  into a symplectic manifold.

This symplectic manifold  $\mathcal{S}_X$  measures the “non-Hamiltonianess” of the vector field  $X$ . The submanifold  $\mathcal{S}_X$  is the classical analogue of von Neumann’s deficiency spaces  $\mathcal{N}_\pm$  for a symmetric operator.

Inspired by the same idea as von Neumann’s theorem, Thm. 5, one way to make  $X$  into a Hamiltonian vector field would be to “remove” this symplectic manifold  $\mathcal{S}_X$  converting it into a Lagrangian submanifold of a bigger space. The details of this construction will be discussed elsewhere.

However the two constructions proposed above are not really addressing the classical analogue of the problem of unitarization of a symmetric operator because they are not “boundary problems”.

The non-Hamiltonian character of the vector field  $X$  above does not come from

any boundary condition for the classical system. Such non-Hamiltonian character is local in the interior of the manifold  $M$  because the Lie derivative appearing on Eq. (96) is defined locally, contrary to what happens with the effect of boundary conditions in quantum evolution as it was discussed in the previous section.

Boundary conditions in classical Hamiltonian systems will be described as follows. Let us consider a classical mechanical system with configuration space again a smooth Riemannian manifold  $\Omega$  with non-empty boundary  $\partial\Omega$ . Now we impose boundary conditions for the free system on  $\Omega$ , but contrary to the discussion in the Introduction, Eq. (1), by means of a non-canonical map  $S: T^*\partial\Omega \rightarrow T^*\partial\Omega$ ,  $S^*\omega_{\partial\Omega} \neq \omega_{\partial\Omega}$ , with  $\omega_{\partial\Omega}$  the canonical symplectic structure on  $T^*\partial\Omega$ .

It is clear that the mechanical effect of such non-canonical boundary condition is going to be related to dissipation of volume density of  $T^*\Omega$  at the boundary. Thus we can think that this volume density is transmitted to a “mirror space” or external space that has been put in contact with the original one through its boundary. Thus, the natural way to recover a symplectic (hence volume-preserving) evolution, would be to double the space by adding a mirror image of  $T^*\Omega$  and pasting the two of them by means of the boundary condition  $S$ . This requires some care because  $S$  is not a map from  $\partial(T^*\Omega)$  into itself, but rather a map between the symplectic boundaries of the two spaces [As94]. As in previous discussions we will not pursue the description of the classical situation leaving it for later developments and we will concentrate on the quantum situation.

It has become clear from the previous comments at the classical level, that a good strategy to restore unitarity for non-self-adjoint extensions of symmetric operators, in particular the Hodge Laplacian, would be to double our state space using a mirror image of the original one and then using the boundary conditions to “paste” the domains of the original operator and its mirror image in such a way that the dissipation introduced by the former will be transmitted to the later [Bo95].

Analytically we will proceed as follows. Let us denote as in Section 3 by  $H^2(\Omega)$  the Sobolev Hilbert space defining the maximal extension of the operator  $-\Delta$ . The boundary data space will be denoted as usual by  $\mathcal{H}_B$  and an elliptic extension of  $-\Delta_0$  will be defined by the subspace  $W \in \mathbf{Gr}$ . In particular we will assume that  $W$  is the graph of a non-self-adjoint operator  $A: \mathcal{L}_+ \rightarrow \mathcal{L}_-$ ,  $\dot{\varphi} = A\varphi$ .

We introduce a mirror Hilbert space  $H^2(\Omega)_{\text{mirror}}$  which is a copy of  $H^2(\Omega)$  and, in the direct sum Hilbert space  $H^2(\Omega) \oplus H^2(\Omega)_{\text{mirror}}$ , we will define an extended operator  $-\Delta_{\text{ext}}$  as follows. In the domain  $H^2(\Omega) \oplus H^2(\Omega)_{\text{mirror}}$ , the operator  $-\Delta_{\text{ext}}$  is the direct sum of  $-\Delta_0 \oplus -\Delta_0$ . Thus the operator  $-\Delta_{\text{ext}}$  with domain  $H_0^2(\Omega) \oplus H_0^2(\Omega)_{\text{mirror}}$  is symmetric.

If we denote now by  $\Psi_{\text{ext}} \in H^2(\Omega) \oplus H^2(\Omega)_{\text{mirror}}$  a vector on the enlarged space, we will denote by  $\Psi$  the projection  $\pi(\Psi_{\text{ext}})$  of  $\Psi_{\text{ext}}$  into its first factor and by  $\Psi_{\text{mirror}}$  the projection  $\pi_2(\Psi_{\text{ext}})$  onto the second factor  $H^2(\Omega)_{\text{mirror}}$ . Then, given  $\Psi_{\text{ext}}$  we will define the ordinary boundary values  $b(\pi_1(\Psi_{\text{ext}})) = (\varphi, \dot{\varphi})$  and the mirror boundary values  $b(\pi_2(\Psi_{\text{ext}})) = b(\psi_{\text{mirror}}) = (\varphi_{\text{mirror}}, \dot{\varphi}_{\text{mirror}})$ .

Then, we define the domain of  $-\Delta_{\text{ext}}$  associated to the operator  $A$  as the space of functions  $\psi_{\text{ext}}$  such that:

$$\dot{\varphi}_{\text{mirror}} = A^\dagger \varphi, \quad \dot{\varphi} = A \varphi_{\text{mirror}}. \quad (97)$$

We shall denote this subspace as  $b^{-1}(W_A)_{\text{ext}}$ .

The following computation shows that  $-\Delta_{\text{ext}}$  is self-adjoint in  $b^{-1}(W_A)_{\text{ext}}$ .

$$\begin{aligned} \langle -\Delta_{\text{ext}} \Psi_{\text{ext}}, \Psi'_{\text{ext}} \rangle &= \langle -\Delta_{\text{ext}}(\Psi, \Psi_{\text{mirror}}), (\Psi', \Psi'_{\text{mirror}}) \rangle \\ &= \langle (-\Delta \Psi, -\Delta \Psi_{\text{mirror}}), (\Psi', \Psi'_{\text{mirror}}) \rangle \\ &= \langle -\Delta \Psi, \Psi' \rangle + \langle -\Delta \Psi_{\text{mirror}}, \Psi'_{\text{mirror}} \rangle \\ &= \langle \Psi, -\Delta \Psi' \rangle + \langle \Psi_{\text{mirror}}, -\Delta \Psi'_{\text{mirror}} \rangle \\ &\quad + \langle \dot{\varphi}, \varphi' \rangle - \langle \varphi, \dot{\varphi}' \rangle + \langle \dot{\varphi}_{\text{mirror}}, \varphi'_{\text{mirror}} \rangle - \langle \varphi_{\text{mirror}}, \dot{\varphi}'_{\text{mirror}} \rangle. \end{aligned}$$

But using the boundary conditions Eq. (97), the last four terms in the previous equation become,

$$\begin{aligned} &\langle \dot{\varphi}, \varphi' \rangle - \langle \varphi, \dot{\varphi}' \rangle + \langle \dot{\varphi}_{\text{mirror}}, \varphi'_{\text{mirror}} \rangle - \langle \varphi_{\text{mirror}}, \dot{\varphi}'_{\text{mirror}} \rangle \\ &= \langle A \varphi_{\text{mirror}}, \varphi' \rangle - \langle \varphi, A \varphi'_{\text{mirror}} \rangle \\ &\quad + \langle A^\dagger \varphi, \varphi'_{\text{mirror}} \rangle - \langle \varphi_{\text{mirror}}, A^\dagger \varphi' \rangle = 0. \end{aligned}$$

Hence the operator is self-adjoint as claimed.

We have proved the following theorem.

**Theorem 14.** *Given the dissipative quantum system defined on a Riemannian manifold  $\Omega$  with non-empty boundary  $\partial\Omega$  by the Hamiltonian  $H_0 = -\frac{1}{2}\Delta_A$ , with  $\Delta_A$  the Bochner Laplacian determined by the metric and a connection  $A$ , and non-self-adjoint elliptic boundary conditions defined by the non-self-adjoint boundary operator  $A$ , there exists an unitarization of the system on the enlarged Hilbert space  $L^2(\Omega) \oplus L^2(\Omega)_{\text{mirror}}$  determined by the boundary conditions given by Eq. (97).*



## 8. Self-adjoint extensions of elliptic operators with symmetry

This section will be devoted to the analysis of the structure and the global properties of self-adjoint extensions of elliptic operators invariant with respect to a Lie group of transformations. As before we will discuss the theory for Dirac operators and the ideas extend in a natural way to higher order differential elliptic operators.

### 8.1. Dirac bundles with symmetry

Let us consider the following geometrical setting. Let  $G$  be a Lie group acting on  $\Omega$  smoothly, i.e., there is a smooth map  $\Phi: G \times \Omega \rightarrow \Omega$  such that  $\Phi(e, x) = x$  for all  $x \in \Omega$ ,  $\Phi(h, \Phi(g, x)) = \Phi(hg, x)$ , for all  $g, h \in G$ ,  $x \in \Omega$ , and  $\Phi(g, x) \in \partial\Omega$  for every  $x \in \partial\Omega$ . As usual the action  $\Phi(g, x)$  will be denoted simply by  $gx$ , and the induced action of  $G$  on  $\partial\Omega$  will be denoted with the same symbol.

The space of orbits of the action will be denoted by  $\Omega/G$  and if the action of  $G$  on  $\Omega$  is proper and free the quotient space  $\Omega/G$  will be a smooth manifold with boundary  $\partial(\Omega/G) = \partial\Omega/G$ . The Riemannian structure  $\eta$  can be chosen to be invariant if the group is compact. In fact, in that case we can average an arbitrary Riemannian structure to obtain an invariant Riemannian structure on  $\Omega$ .

The action of the group  $G$  lifts naturally to the tangent bundle  $T\Omega$  and the action is given by the tangent maps of the diffeomorphisms defined by the group elements  $g \in G$  and the corresponding action on the space of vector fields on  $\Omega$  will be denoted by  $g_*X$ ,  $X \in \mathfrak{X}(\Omega)$ .

Let us consider as in the previous sections a Dirac bundle  $\pi: S \rightarrow \Omega$  such that there exists a lifting of the action of  $G$  on  $\Omega$  to the total space  $S$  of the bundle, i.e., there exists an action map  $\Psi: G \times S \rightarrow S$  such that it commutes with the natural projection maps, that is,

$$\pi \circ \Psi = \Phi \circ \pi,$$

and the action of  $g \in G$  on  $S$  maps linearly the fibre over  $x$  into the fibre over  $gx$ . Thus, the action  $\Psi$  preserves the boundary bundle  $S_{\partial\Omega}$  over  $\partial\Omega$ . We will assume that we can choose the Hermitean structure on the Dirac bundle  $S$  to be  $G$  invariant, i.e.,

$$(g\xi, g\zeta)_{gx} = (\xi, \zeta)_x, \quad \forall g \in G, \quad \xi, \zeta \in S_x,$$

and the group  $G$  will be represented unitarily on the bundle  $S$ , as well as the Hermitean connection  $\nabla$ , that is, because the group  $G$  acts in the space of sections  $\Gamma(S)$  as  $(g \cdot \sigma)(x) = \Psi(g, \sigma(\Phi(g^{-1}, x)))$ ,  $x \in \Omega$ ,  $g \in G$ , then

$$\nabla_{g_*X}(g \cdot \sigma) = g \cdot (\nabla_X \sigma), \quad \forall \sigma \in \Gamma(S), \quad X \in \mathfrak{X}(\Omega), \quad g \in G.$$

As the Riemannian metric  $\eta$  is  $G$ -invariant, the action of the group lifts to the Clifford algebra bundle  $\text{Cl}(\Omega)$  over  $\Omega$ . The action  $\rho$  of the Clifford algebra bundle  $\text{Cl}(\Omega)$  on the Dirac bundle  $S$  defines a homomorphism of algebra bundles  $\rho: \text{Cl}(\Omega) \rightarrow \text{End}(S)$ , where  $\text{End}(S)$  denotes the algebra bundle of endomorphisms

of the vector bundle  $S$ . The group  $G$  acts on the vector bundle  $S$  by endomorphisms, thus this action extends to the algebra bundle  $\text{End}(S)$  in a natural way, that is, if  $h: S \rightarrow S$  is a bundle homomorphism, then  $h^g = g^{-1} \circ h \circ g$ ,  $g \in G$ . Thus we have two  $G$ -spaces,  $\text{Cl}(\Omega)$  and  $\text{End}(S)$  and a map  $\rho$  between them, then if the group  $G$  is compact, we can choose this map to be equivariant by averaging. In fact let

$$\rho_G(u) = \int_G \rho(gu)^{g^{-1}} d\mu_G(g),$$

where  $d\mu_g$  denotes (the normalized Haar measure on the group  $G$ . Then,

$$\begin{aligned} \rho_G(hu) &= \int_G \rho(ghu)^{g^{-1}} d\mu_G(g) = \int_G \rho(ku)^{kh^{-1}} d\mu_G(k) = \int_G \rho(ku)^{k^{h^{-1}}} d\mu_G(k) \\ &= \left( \int_G \rho(ku)^k d\mu_G(k) \right)^{h^{-1}} = \rho_G(u)^{h^{-1}}. \end{aligned}$$

Finally, if the group  $G$  is compact the connection  $\nabla$  in  $S$  can be chosen to be equivariant by averaging again a given connection. It is easy to check that if the given connection were verifying the derivation property (5), then the averaged connection will satisfy it again.

Summarizing the previous discussion, we have arrived at the following result.

**Proposition 15.** *Let  $S$  be a Dirac bundle over the Riemannian manifold with boundary  $\Omega$  and let  $G$  be a compact Lie group acting on the bundle  $S$  by bundle isomorphisms, then there exists a Dirac bundle structure on  $S$  which is  $G$ -invariant. Besides the Dirac operator constructed using it will commute with the action of  $G$  and is topologically equivalent to the initial one.*

Proof. It is immediate from the previous considerations and the fact that the space of connections and metrics is contractible, then there exists a continuous path  $\mathcal{D}_t$  connecting the Dirac operator  $\mathcal{D}$  and the averaged one  $\mathcal{D}_{inv}$ .  $\square$

## 8.2. The quotient Dirac operator

Under the conditions stated in Prop. 15 we have constructed an equivariant Dirac operator, that we simply denote again by  $\mathcal{D}$ . If the action of the group  $G$  on  $S$  is “good enough”, e.g., proper and free, then the quotient total space  $S/G$  will be a smooth bundle over the quotient manifold  $\Omega/G$  with smooth boundary  $\partial\Omega/G$ . Moreover the structures on  $S$  will be related to the corresponding structures on the quotient and the bundle  $S/G \rightarrow \Omega/G$  will be again a Dirac bundle with Dirac operator  $\mathcal{D}_G$ .

We will denote by  $\pi_G$  the projection map between the quotient spaces  $S/G$  and  $\Omega/G$  above defined as:  $\pi_G([\xi]) = [\pi(\xi)]$ , where  $[\xi]$  denotes the orbit of  $\xi \in S$  under the action of  $G$  and, similarly,  $[x]$  is the orbit of  $x$  in  $\Omega$ . The Dirac bundle  $\pi_G: S/G \rightarrow \Omega/G$  will be called the quotient Dirac bundle.

The space of sections  $\Gamma(S/G)$  of the quotient Dirac bundle  $S/G$  are in one-to-one correspondence with the space of equivariant sections of  $S$  under the action of  $G$ , that is:  $\Gamma(S/G) = \Gamma(S)^G$ , with

$$\Gamma(S)^G = \{\sigma \in \Gamma(S) \mid g \cdot \sigma = \sigma\}.$$

Notice that if  $\sigma \in \Gamma(S)^G$  we may define  $\tilde{\sigma}([x]) = \sigma(x)$  for all  $[x] \in \Omega/G$ . then  $\tilde{\sigma}$  defines a section of  $E/G$  as it satisfies that  $[\sigma([x])] = [\sigma([x'])]$  whenever  $[x] = [x']$ . On the other hand, if  $\tilde{\sigma}: \Omega/G \rightarrow S/G$  is a section, then we may define  $\sigma(x) = \int_G g^{-1}(\tilde{\sigma}(\pi(x))) d\mu_G(g)$ ,  $x \in \Omega$  which is an invariant section of  $S$ .

Because of the  $G$ -equivariance of the Dirac operator  $\not{D}$  on  $S$ , it will induce an operator on the quotient space that we will denote by  $\not{D}/G$ . Actually, notice that if  $\sigma \in \Gamma(S)^G$ , then

$$\not{D}g \cdot \sigma = e_i \cdot \nabla_{e_i} g \cdot \sigma = g \cdot \not{D}\sigma \quad (98)$$

and then it makes sense to define

$$\not{D}_G[\sigma] = \not{D}([\sigma]), \quad \forall [\sigma] \in \Gamma.$$

**Remark 16.** It is clear that under the previous conditions for the action of  $G$  on  $S$ , then  $\not{D}/G = \not{D}_G$ . We shall remark here that even if the quotient space  $S/G$  fails to be a smooth bundle over a smooth manifold  $\Omega/G$ , this will happen for instance if the action of  $G$  is not free, the induced operator  $\not{D}/G$  will still be defined as the following discussion shows.

The group  $G$  acts naturally on the space of smooth sections of  $S$ , as indicated above, i.e.,

$$(g \cdot \xi)(x) = g(\xi(g^{-1}x)), \quad \forall g \in G, x \in \Omega. \quad (99)$$

By continuity this action extends unitarily to the spaces of sections  $H_0^1(\Omega, S)$ ,  $H^1(\Omega, S)$  and  $L^2(\Omega, S)$  because:

$$\begin{aligned} \langle g \cdot \xi, g \cdot \zeta \rangle &= \int_{\Omega} (g \cdot \xi(x), g \cdot \zeta(x))_x \text{vol}_{\eta}(x) \\ &= \int_{\Omega} (\xi(g^{-1}x), \zeta(g^{-1}x))_x \text{vol}_{\eta}(x) \\ &= \int_{\Omega} (\xi(x), \zeta(x))_x \text{vol}_{\eta}(x) = \langle \xi, \zeta \rangle, \end{aligned}$$

where we have used that  $G$  acts by isometries of  $\eta$ , then it preserves the volume form  $\text{vol}_{\eta}$ , hence the Jacobian of the diffeomorphism  $g$  will be trivial. Besides  $g$  acts by unitary transformations on the hermitian bundle  $S$ . Thus, the Hilbert spaces of sections before support unitary representations of the group  $G$ .

Similarly, the boundary data Hilbert space  $\mathcal{H}_D$  will also define a unitary representation of the group  $G$ . The boundary map  $b$  is equivariant because the pull-back

60 *M. Asorey, A. Ibort, G. Marmo*

map  $i: \partial\Omega \rightarrow \Omega$  commutes with the action of  $G$  and the following diagramme is commutative

$$\begin{array}{ccc} H^1(\Omega, S) & \xrightarrow{V(g)} & H^1(\Omega, S) \\ \downarrow & & \downarrow \\ H^{1/2}(\partial\Omega, S_{\partial\Omega}) & \xrightarrow{v(g)} & H^{1/2}(\partial\Omega, S_{\partial\Omega}) \end{array}, \quad (100)$$

where  $V(g): H^1(\Omega, S) \rightarrow H^1(\Omega, S)$  denotes the unitary representation of the group  $G$  defined by Eq. (99) and  $v(g): H^{1/2}(\partial\Omega, S_{\partial\Omega}) \rightarrow H^{1/2}(\partial\Omega, S_{\partial\Omega})$  is the corresponding unitary representation induced in the restriction of the Dirac bundle  $S$  to the boundary (see next section, Sect. 8.3, for more details).

We will not pursue this analysis here, but it is obvious that the multiplicities of the irreducible representations of  $G$  contained in the Hilbert space  $H^1(S)$  will be related to the multiplicities of the corresponding ones in the boundary Hilbert space  $\mathcal{H}_D$ . More elaborate comments on this will be done later.

Now we will define the quotient operator  $\mathcal{D}/G$ . Let  $\Gamma_0(S)^G$  and  $\Gamma(S)^G$  be the subspaces of smooth invariant sections of  $S$  of  $\Gamma_0(S)$  and  $\Gamma(S)$ , the spaces of compact supported smooth sections of  $S$  and smooth sections of  $S$ , respectively. Clearly, this amounts to  $\xi$  be a fixed point for the action of  $G$  on  $\Gamma(S)$ .

Then we will define  $\mathcal{D}/G$  as a linear map  $\Gamma_0(S)^G \rightarrow \Gamma_0(S)^G$  by means of

$$(\mathcal{D}/G)(\xi) = \mathcal{D}(\xi), \quad \forall \xi \in \Gamma_0^G(S).$$

Notice that because  $\mathcal{D}$  is a differential operator, hence local, and Eq. (98), then  $(\mathcal{D}/G)(\xi) \in \Gamma_0(S)^G$ .

Clearly the operator  $\mathcal{D}/G$  is symmetric on the domain  $\Gamma_0(S)^G$  and we can search for its self-adjoint extensions. Of course,  $\Gamma_0(S)^G$  is not dense in  $H^1(\Omega, S)$  but it is dense in the intersection of the  $L^2$ -closure of  $\Gamma(S)^G$  and  $H^1(S)$ . Such space, denoted in what follows by  $H^1(S)^G$ , will play the role of the Hilbert space of sections of Sobolev class 1 in the quotient bundle space  $S/G$ . Notice that  $H^1(S)^G$  coincides with the subspace of fixed sections under the action of  $G$  in  $H^1(S)$ . Thus we have,

**Proposition 17.** *If we denote by  $\text{Fix}_G(H^1(S))$  the fixed set of the unitary action  $V(g)$  of  $G$  in  $H^1(\Omega, S)$ , then,*

$$\text{Fix}_G(H^1(S)) = H^1(S)^G,$$

*and similarly for  $H_0^1(\Omega, S)$ . Moreover, if the quotient spaces  $S/G$ ,  $\Omega/G$  are smooth manifolds and the canonical projection is a smooth submersions, then*

$$H^1(S)^G \cong H^1(S/G),$$

*where the later identification means that there is a natural unitary transformation from the Hilbert space  $H^1(S)^G$  and the Hilbert space of order 1 Sobolev sections of the bundle  $S/G \rightarrow \Omega/G$ .*

Once the quotient operator  $\not{D}/G$  has been defined and it has been shown to be symmetric in a dense domain of the Hilbert space  $H^1(\Omega, S)^G$  we can, as we did for the Dirac operator  $\not{D}$ , compute and characterize all its selfadjoint extensions. Of course, as it was discussed before, if the action of  $G$  defines a quotient Dirac bundle  $S/G \rightarrow \Omega/G$ , the space  $H^1(\Omega, S)^G$  is precisely the space  $H^1(S/G)$  of sections of the quotient bundle, and the quotient operator  $\not{D}/G$  is precisely the Dirac operator  $\not{D}_G$  in the quotient bundle, thus using the results and the discussion in Section 2.3, Thm. 2, its self-adjoint extensions are given by the self-adjoint Grassmannian  $\mathcal{M}(\not{D}_G)$  on the boundary Hilbert space  $\mathcal{H}_{\not{D}_G} = H^{1/2}(\partial\Omega, S_{\partial\Omega})$  defined on the boundary  $\partial\Omega/G$  and the problem will be solved.

In spite of this, we would like to characterize such self-adjoint extensions in terms of self-adjoint extensions for  $\not{D}$  on  $\Omega$ , i.e., we are asking how to obtain  $\mathcal{M}(\not{D}_G)$  directly from  $\mathcal{M}(\not{D})$ . Apart from the intrinsic interest of being able to compute things in quotient spaces without having to go to the quotient, avoiding the inherent difficulties of taking quotients, this approach to the problem has the advantage of providing an effective method to construct the self-adjoint extensions of the quotient Dirac operator  $\not{D}/G$  when  $S/G$  is not a manifold, a situation which is often found in all sort of problems.

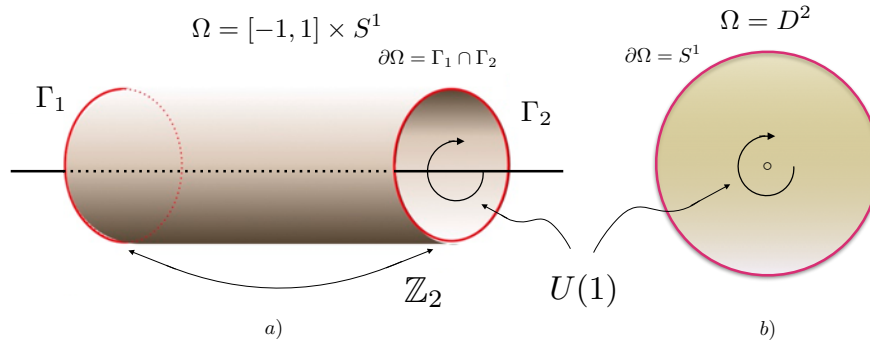


Fig. 1. The cylinder (a) and disk (b) with the groups  $U(1)$  and  $\mathbb{Z}_2$  acting on them.

For instance, consider the following two simple examples. Let  $\Omega = S^1 \times [0, 1]$  be the cylinder with boundary  $\partial\Omega = S^1 \times \{0\} \cup S^1 \times \{1\}$  and consider the natural action of the group  $U(1)$  on  $\Omega$  by rotations along the symmetry axis of the cylinder (see Fig. 1). Then the quotient space  $\Omega/U(1)$  is clearly the smooth manifold with boundary  $[0, 1]$ , and we could expect that the  $U(1)$ -invariant self-adjoint extensions of a Dirac operator defined on a given Dirac bundle over  $\Omega$  will correspond to the self-adjoint extensions of the Dirac operator defined by the projection of that bundle to  $[0, 1]$ . It is easy to check that if  $S$  is a complex line bundle (the Spin bundle of the manifold), then  $\mathcal{M}(\not{D}_{U(1)}) \cong U(1)$ .

Consider now, instead of the cylinder the unit disk. That is,  $\Omega = \{z \in \mathbb{C} \mid |z| \leq 1\}$  with boundary  $\partial\Omega = S^1$ . Consider now the natural action of  $U(1)$  on  $\Omega$  by complex multiplication, i.e., rotation around the origin in  $\mathbb{C}$ . The action of  $U(1)$  is not free, however the quotient space is a smooth manifold with boundary,  $[0, 1]$  again. What happens to the self-adjoint extensions of the quotient operator now? Do we obtain all self-adjoint extensions of  $\mathcal{D}_{U(1)}$  by looking at the  $U(1)$ -invariant ones in  $\Omega$ ? Clearly no, new self-adjoint extensions on the quotient space arise because of the non-trivial nature of the action of the group  $z$  (the origin is a fixed point for the action).

We will analyse in what follows these matters. We will restate some of the notions introduced above concerning Dirac operators in a slightly more general context, and we will proceed then to a direct construction of the ‘quotient’ self-adjoint Grassmannian.

### 8.3. Unitaries at the boundary and $G$ -invariance

Let us consider now a Hermitean bundle  $\pi: E \rightarrow \Omega$ , with  $(\Omega, \eta)$  a Riemannian manifold with smooth boundary  $\partial\Omega$ .

Let  $G$  be a Lie group and  $V: G \rightarrow \mathcal{U}(L^2(\Omega, E))$  be a continuous unitary representation of  $G$ , on the Hilbert space of square integrable sections of  $E \rightarrow \Omega$ , i.e., for any  $\Phi \in L^2(\Omega, E)$  the map

$$G \ni g \mapsto V(g)\Phi$$

is continuous in the  $L^2$ -norm  $\|\Phi\|^2 = \int_{\Omega} \|\Phi(x)\|^2 \text{vol}_{\eta}$ .

Notice that if the unitary representation  $V$  leaves invariant the subspace  $H^1(\Omega, E)$ , i.e.,  $V(g)H^1(\Omega) \subset H^1(\Omega)$ , and it leaves invariant the quadratic form  $Q(\Phi) = \|\nabla\Phi\|^2$ , where  $\nabla$  is a Hermitean connection on  $E$  and  $Q$  is defined on Neumann’s domain  $H^1(\Omega, E)$ , (we call  $Q$  with such domain the Neumann’s quadratic form), that is

$$Q(V(g)\Phi) = Q(\Phi) \quad \forall g \in G, \Phi \in H^1(\Omega, E),$$

then  $V$  defines also a continuous unitary representation on  $\mathcal{H}^1(\Omega)$  with its corresponding Sobolev scalar product (see for instance [Ib14c]). Now we can extend the property of equivariant Dirac operators expressed by Eq. (100), that can be used also to study self-adjoint extensions of Laplace operators.

**Definition 18.** *The representation  $V: G \rightarrow \mathcal{U}(L^2(\Omega, E))$  has a trace (or is traceable) along the boundary  $\partial\Omega$ , if it leaves invariant Neumann’s quadratic form  $Q$  and there exists another continuous, unitary representation  $v: G \rightarrow \mathcal{U}(L^2(E_{\partial\Omega}))$  such that*

$$b(V(g)\Phi) = v(g)\gamma(\Phi), \tag{101}$$

for all  $\Phi \in H^1(\Omega, E)$  and  $g \in G$  or, in other words, that the following diagram is

commutative:

$$\begin{array}{ccc} H^1(\Omega, E) & \xrightarrow{V(g)} & H^1(\Omega, E) \\ b \downarrow & & \downarrow b \\ H^{1/2}(\partial\Omega, E_{\partial\Omega}) & \xrightarrow{v(g)} & H^{1/2}(\partial\Omega, E_{\partial\Omega}) \end{array}$$

We will call  $v$  the trace of the representation  $V$ .

Notice that if the representation  $V$  is traceable, its trace  $v$  is unique. It is not difficult to prove the following theorem: (see the proof in the case of Laplace operators in [Ib14c]).

**Theorem 19.** *Let  $G$  be a Lie group,  $\pi: E \rightarrow \Omega$  a Dirac bundle over  $\Omega$  and  $\not{D}$  a Dirac operator on it. Let  $V: G \rightarrow \mathcal{U}(L^2(\Omega, E))$  be a traceable continuous, unitary representation of  $G$  with unitary trace  $v: G \rightarrow \mathcal{U}(L^2(\partial\Omega, E_{\partial\Omega}))$  along the boundary  $\partial\Omega$ . Denote by  $(\not{D}_U, \mathcal{D}_U)$  the self-adjoint extension of the Dirac operator  $\not{D}$  determined by the unitary operator  $U: H^{1/2}(\partial\Omega, E_{\partial\Omega}) \rightarrow H^{1/2}(\partial\Omega, E_{\partial\Omega})$ . Then we have that  $[v(g), U] = 0$  for all  $g \in G$  iff  $\not{D}_U$  is  $G$ -invariant.*

#### 8.4. Examples: Groups acting by isometries

In this section we will discuss some examples with unitaries which satisfy the conditions mentioned in the statements above derived by actions of groups by unitary transformations of the bundle  $E$  covering isometries on  $\Omega$ .

Thus, assume as in Section 8.1, that the group  $G$  acts smoothly by isometries on the Riemannian manifold  $(\Omega, \partial\Omega, \eta)$  and this action can be lifted to an unitary action on the bundle  $\pi: E \rightarrow \Omega$ . Any  $g \in G$  specifies a bundle isomorphism  $g_E: E \rightarrow E$  such that  $(g_E \cdot \xi, g_E \cdot \zeta) = (\xi, \zeta)$ , for all  $\xi, \zeta \in E$  and  $(\cdot, \cdot)$  denotes the inner product along the fibers of  $E$ . The element  $g \in G$  defines also a diffeomorphism  $g_\Omega: \Omega \rightarrow \Omega$  such that  $\pi(g_E \cdot \xi) = g_\Omega \cdot \pi(\xi)$ . Moreover, we have that  $g_\Omega^* \eta = \eta$ , where  $g_\Omega^*$  stands for the pull-back by the diffeomorphism  $g$ . These diffeomorphisms restrict to isometric diffeomorphisms on the Riemannian manifold at the boundary  $(\partial\Omega, \partial\eta)$  (see, e.g., [Ab88, Lemma 8.2.4]),

$$(g|_{\partial\Omega})^* \partial\eta = \partial\eta,$$

hence the action on  $E$  restricts to an action on  $E_{\partial\Omega}$ , the pull-back of the bundle  $E$  to the boundary  $\partial\Omega$ . These actions of the group  $G$  induce unitary representations of the group on the space of square integrable sections of the bundles  $E \rightarrow \Omega$  and  $E_{\partial\Omega} \rightarrow \partial\Omega$ . In fact, consider the following representations:

$$\begin{aligned} V: G &\rightarrow \mathcal{U}(L^2(\Omega, E)), & V(g)\Phi &= g_E \cdot \Phi \circ g_\Omega^{-1}, \Phi \in L^2(\Omega, E), \\ v: G &\rightarrow \mathcal{U}(L^2(\partial\Omega, E_{\partial\Omega})), & v(g)\varphi &= g_E|_{E_{\partial\Omega}} \cdot \varphi \circ (g|_{\partial\Omega})^{-1}, \varphi \in L^2(\partial\Omega, E_{\partial\Omega}). \end{aligned}$$

Then a simple computation shows that,

$$\langle V(g^{-1})\Phi, V(g^{-1})\Psi \rangle = \langle \Phi, \Psi \rangle,$$

where we have used the change of variables formula and the fact that isometric diffeomorphisms preserve the Riemannian volume, i.e.,  $g^*d\mu_\eta = d\mu_\eta$ . The result for the boundary is proved similarly. The induced actions are related with the boundary map as in Eq. (18),  $(V(g)\Phi) = v(g)b(\Phi)$ ,  $g \in G$ ,  $\Phi \in H^1(\Omega)$ , and therefore the unitary representation  $V$  is traceable along the boundary of  $\Omega$  with trace  $v$ .

Moreover we have that Neumann's quadratic form  $Q$  is  $G$ -invariant.

**Proposition 20.** *Let  $G$  be a Lie group that acts by unitary bundle isomorphisms on the Hermitean bundle  $\pi: E \rightarrow \Omega$  over the Riemannian manifold with boundary  $(\Omega, \partial\Omega, \eta)$  and let  $V: G \rightarrow \mathcal{U}(L^2(\Omega, E))$  be the associated unitary representation. Then, Neumann's quadratic form  $Q_N(\Phi) = \langle \nabla \Phi, \nabla \Phi \rangle$  with domain  $H^1(\Omega, E)$  is  $G$ -invariant, where  $\nabla$  is a  $G$ -invariant connection.*

**Proof.** Let us consider the simpler case of a trivial line bundle over  $\Omega$  and trivial unitary action of  $G$  along the fibres. Then the connection  $\nabla$  is trivial. The general case is a trivial extension.

First notice that the pull-back of a diffeomorphism commutes with the action of the exterior differential. Then we have that

$$d(V(g^{-1})\Phi) = d(g^*\Phi) = g^*d\Phi.$$

Hence

$$\begin{aligned} \langle d(V(g^{-1})\Phi), d(V(g^{-1})\Psi) \rangle &= \int_{\Omega} \eta^{-1}(g^*d\Phi, g^*d\Psi) d\mu_\eta \\ &= \int_{\Omega} g^*(\eta^{-1}(d\Phi, d\Psi)) g^*d\mu_\eta \\ &= \int_{g\Omega} \eta^{-1}(d\Phi, d\Psi) d\mu_\eta \\ &= \langle d\Phi, d\Psi \rangle, \end{aligned} \tag{102a}$$

where in the second inequality we have used that  $g: \Omega \rightarrow \Omega$  is an isometry and therefore

$$\eta^{-1}(g^*d\Phi, g^*d\Psi) = g^*\eta^{-1}(g^*d\Phi, g^*d\Psi) = g^*(\eta^{-1}(d\Phi, d\Psi)).$$

The equations (102) guaranty also that  $V(g)H^1(\Omega) = H^1(\Omega)$  since  $V(g)$  is a unitary operator in  $L^2(\Omega)$  and the norm  $\sqrt{\|d\cdot\|^2 + \|\cdot\|^2}$  is equivalent to the Sobolev norm of order 1.  $\square$

**Remark 21.** Before making explicit the previous structures in concrete examples we notice that the previous discussion works in a similar way with the covariant Laplacian  $\Delta_A$  discussed in Section 3. Thus if we are given a group acting by unitary bundle isomorphisms on an Hermitean bundle  $E \rightarrow \Omega$  (and by isometric diffeomorphisms on the Riemannian manifold  $\Omega$ ), then any unitary operator  $U$  at the boundary, (that in addition satisfies the conditions of possessing gap and being admissible, [Ib14c], that guarantee that the quadratic form constructed from the operator  $\nabla$



with boundary conditions dictated by  $U$ , read more about self-adjoint extensions determined by quadratic forms in [Ib14] and [Ib15] this volume), and that verifies the commutation relations of Theorem 19 describes a  $G$ -invariant quadratic form. The closure of this quadratic form characterizes uniquely a  $G$ -invariant self-adjoint extension of the Laplace-Beltrami operator.

**Example 22.** Discrete and compact groups of isometries

We will discuss now two particular examples of  $G$ -invariant quadratic forms. In the first example we are considering a situation where the symmetry group is a finite, discrete group. In the second one we consider  $G$  to be a compact Lie group.

- (1) Let  $\Omega$  be the cylinder  $[-1, 1] \times [-1, 1]/\sim$ , where  $\sim$  is the equivalence relation  $(x, 1) \sim (x, -1)$ . The boundary  $\partial\Omega$  is the disjoint union of the two circles  $\Gamma_1 = \{-1\} \times [-1, 1]/\sim$  and  $\Gamma_2 = \{1\} \times [-1, 1]/\sim$ , (see Figure 1 (a)). Let  $\eta$  be the euclidean metric on  $\Omega$ . Now let  $G = \mathbb{Z}_2 = \{e, f\}$  be the discrete, abelian group of two elements and consider the following action in  $\Omega$ :

$$\begin{aligned} e : (x, y) &\rightarrow (x, y) , \\ f : (x, y) &\rightarrow (-x, y) . \end{aligned}$$

The induced action at the boundary is

$$\begin{aligned} e : (\pm 1, y) &\rightarrow (\pm 1, y) , \\ f : (\pm 1, y) &\rightarrow (\mp 1, y) . \end{aligned}$$

Clearly  $G$  transforms  $\Omega$  onto itself and preserves the boundary. Moreover, it is easy to check that  $f^*\eta = \eta$ .

Since the boundary  $\partial\Omega$  consists of two disjoint manifolds  $\Gamma_1$  and  $\Gamma_2$ , the Hilbert space of the boundary is  $L^2(\partial\Omega, E) = L^2(\Gamma_1, E) \oplus L^2(\Gamma_2, E)$ . Any  $\Phi \in L^2(\partial\Omega, E)$  can be written as

$$\Phi = \begin{pmatrix} \Phi_1(y) \\ \Phi_2(y) \end{pmatrix}$$

with  $\Phi_i \in L^2(\Gamma_i, E)$ . A nontrivial action on  $L^2(\partial\Omega)$  is given by

$$v(f) \begin{pmatrix} \Phi_1(y) \\ \Phi_2(y) \end{pmatrix} = \begin{pmatrix} 0 & v \\ v^\dagger & 0 \end{pmatrix} \begin{pmatrix} \Phi_1(y) \\ \Phi_2(y) \end{pmatrix} ,$$

where  $v : L^2(\Gamma_2, E) \rightarrow L^2(\Gamma_1, E)$  is a unitary operator. The set of unitary operators that describe the closable quadratic forms as defined in the previous section is given by suitable unitary operators

$$U = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} ,$$

with  $U_{ij} = L^2(\Gamma_j) \rightarrow L^2(\Gamma_i)$ . According to Theorem 19 the unitary operators commuting with  $v(f)$  will lead to  $G$ -invariant quadratic forms. Imposing

$[v(f), U] = 0$ , we get the conditions

$$\begin{aligned} U_{12} &= vU_{12}v, \\ U_{22} &= v^\dagger U_{11}v. \end{aligned}$$

Obviously there is a wide class of unitary operators, i.e., boundary conditions, that will be compatible with the symmetry group  $G$ . We will consider next two particular classes of boundary conditions. First, consider the following unitary operators

$$U = \begin{bmatrix} e^{i\beta_1} \mathbb{I}_1 & 0 \\ 0 & e^{i\beta_2} \mathbb{I}_2 \end{bmatrix}, \quad (103)$$

where  $\beta_i \in C^\infty(S^1, [-\pi + \delta, \pi - \delta] \cup \{\pi\})$  for some  $\delta > 0$ . Moreover, this choice of unitary matrices corresponds to select Robin boundary conditions of the form:

$$b\left(-\frac{d\Phi}{dx}\right)\Big|_{\Gamma_1} = -\tan(\beta_1/2)b(\Phi)|_{\Gamma_1}; \quad b\left(\frac{d\Phi}{dx}\right)\Big|_{\Gamma_2} = -\tan(\beta_2/2)b(\Phi)|_{\Gamma_2}. \quad (104)$$

The  $G$ -invariance condition above imposes  $\beta_1 = \beta_2$ . Notice that when  $\beta_1 \neq \beta_2$  we can obtain meaningful self-adjoint extensions of the Laplace-Beltrami operator that, however, will not be  $G$ -invariant.

We can also consider unitary operators of the form

$$U = \begin{bmatrix} 0 & e^{i\alpha} \\ e^{-i\alpha} & 0 \end{bmatrix}, \quad (105)$$

where  $\alpha \in C^\infty(S^1, [0, 2\pi])$ . In this case the unitary matrix corresponds to select so-called quasi-periodic boundary conditions, cf., [As83], i.e.,

$$b(\Phi)|_{\Gamma_1} = e^{i\alpha}b(\Phi)|_{\Gamma_2}, \quad b\left(-\frac{d\Phi}{dx}\right)\Big|_{\Gamma_1} = e^{i\alpha}b\left(\frac{d\Phi}{dx}\right)\Big|_{\Gamma_2}.$$

The  $G$ -invariance condition imposes  $e^{i\alpha} = e^{-i\alpha}$  and therefore among all the quasi-periodic conditions only the periodic ones,  $\alpha \equiv 0$ , are compatible with the  $G$ -invariance.

- (2) Let  $\Omega$  be the unit, upper hemisphere centered at the origin. Its boundary  $\partial\Omega$  is the unit circle on the  $z = 0$  plane. Let  $\eta$  be the induced Riemannian metric from the euclidean metric in  $\mathbb{R}^3$ . Consider the compact Lie group  $G = SO(2)$  that acts by rotation around the  $z$ -axis. If we use polar coordinates on the horizontal plane, then the boundary  $\partial\Omega$  is isomorphic to the interval  $[0, 2\pi]$  with the two endpoints identified. We denote by  $\theta$  the coordinate parameterizing the boundary and the boundary Hilbert space is  $L^2(S^1)$ .

Let  $\varphi \in H^{1/2}(\partial\Omega)$  and consider the action on the boundary by a group element  $g_\alpha \in G$ ,  $\alpha \in [0, 2\pi]$ , given by

$$v(g_\alpha^{-1})\varphi(\theta) = \varphi(\theta + \alpha).$$

To analyze what are the possible unitary operators that lead to  $G$ -invariant quadratic forms it is convenient to use the Fourier series expansions of the elements in  $L^2(\partial\Omega)$ . Let  $\varphi \in L^2(\partial\Omega)$ , then

$$\varphi(\theta) = \sum_{n \in \mathbb{Z}} \hat{\varphi}_n e^{in\theta},$$

where the coefficients of the expansion are given by

$$\hat{\varphi}_n = \frac{1}{2\pi} \int_0^{2\pi} \varphi(\theta) e^{-in\theta} d\theta.$$

We can therefore consider the induced action of the group  $G$  as a unitary operator on  $\ell_2$ , the Hilbert space of square summable sequences. In fact we have that:

$$\begin{aligned} (v(\widehat{g_\alpha^{-1}})\varphi)_n &= \frac{1}{2\pi} \int_0^{2\pi} \varphi(\theta + \alpha) e^{-in\theta} d\theta \\ &= \sum_{m \in \mathbb{Z}} \hat{\varphi}_m e^{im\alpha} \int_0^{2\pi} \frac{e^{i(m-n)\theta}}{2\pi} d\theta = e^{in\alpha} \hat{\varphi}_n. \end{aligned}$$

This shows that the induced action of the group  $G$  is a unitary operator in  $\mathcal{U}(\ell_2)$  that acts diagonally in the Fourier series expansion. More concretely, we can represent it as  $v(\widehat{g_\alpha^{-1}})_{nm} = e^{in\alpha} \delta_{nm}$ . From all the possible unitary operators acting on the Hilbert space of the boundary, only those whose representation in  $\ell_2$  commutes with the above operator will lead to  $G$ -invariant quadratic forms (cf., Theorem 19). Since  $v(\widehat{g_\alpha^{-1}})$  acts diagonally on  $\ell_2$  it is clear that only operators of the form  $\hat{U}_{nm} = e^{i\beta n} \delta_{nm}$ ,  $\{\beta_n\}_n \subset \mathbb{R}$ , will lead to  $G$ -invariant quadratic forms.

As a particular case we can consider that all the parameters are equal, i.e.,  $\beta_n = \beta$ ,  $n \in \mathbb{Z}$ . In this case it is clear that  $(\bar{U}\varphi)_n = e^{i\beta} \hat{\varphi}_n$ , which gives the following admissible unitary with spectral gap at  $-1$ :

$$U\varphi = e^{i\beta} \varphi.$$

This shows that the unique Robin boundary conditions compatible with the  $SO(2)$ -invariance are those that are defined with a constant parameter along the boundary, i.e.,

$$b\left(\frac{d\Phi}{d\nu}\right) = -\tan(\beta/2)b(\Phi), \quad \beta \in [0, 2\pi], \quad (106)$$

where  $\nu$  stands for normal vector field pointing outwards to the boundary.

### 8.5. Reduction of symplectic manifolds by fixed sets and the reduced elliptic Grassmannian

This construction of the reduced self-adjoint Grassmannian, i.e., the space of elliptic self-adjoint extensions of the quotient Dirac operator, will be inspired by a natural construction in symplectic geometry that we will discuss first.

Let  $M$  be a symplectic manifold with symplectic form  $\omega$  and  $G$  a compact group acting by symplectomorphisms on  $M$ . There is a well developed and very successful way of removing the symmetry degrees of freedom of  $M$  under the symmetry group  $G$  known as symplectic reduction (more specifically Marsden-Weinstein reduction in this particular case, see for instance [Ca14, Ch. 7.4] and references therein).

However this scheme is not appropriate for the situation we are considering. In fact, what we need is another reduction scheme which is based on the properties of the singular part of  $M$  with respect to the action of  $G$  (see Section 9 for more details on the stratified structure of  $M$ ). As usual we will denote by  $G_x$  the isotropy group of  $x \in M$ . Then the orbit  $G \cdot x$  through  $x$  is diffeomorphic to the homogeneous space  $G/G_x$ . Two points  $x, y \in M$  are said to lie in the same stratum  $\Sigma$  if the isotropy groups  $G_x$  and  $G_y$  are conjugate in  $G$ . Thus, the points in the same orbit are in the same stratum, but other points in different orbits can be in the same stratum too. In fact, it is easy to see that the strata of  $M$  are  $G$ -invariant and thus they are union of orbits.

There is a natural map from the space of strata into the space of orbits of  $G$  acting by conjugation on its lattice of subgroups. In the space of strata there are two distinguished ones: the maximal stratum  $M_{\text{reg}}$ , which is the union of orbits with minimal isotropy group (when the action is effective, this is the set of points where the group has a locally free action); and the minimal stratum,  $M_{\text{min}}$ , made of the fixed points of the action. If the action is totally ineffective, i.e., trivial, this stratum is the manifold itself.

The manifold  $M/G$  is a stratified manifold too. The strata of the orbit space are in one-to-one correspondence with the strata of  $M$ . The set  $M/G$  decomposes in this way in a disjoint union of smooth manifolds  $S_\alpha$ ,  $M/G = \cup_\alpha S_\alpha$ , where  $\alpha$  labels the strata in  $M$ . The canonical projection  $\pi: M \rightarrow M/G$  is a smooth submersion on each strata. Thus  $\pi^{-1}(S_{\text{min}}) = \text{Fix}_G(M)$  is a smooth submanifold (possibly non connected) of  $M$ .

We will concentrate now in this minimal stratum  $\text{Fix}_G(M)$  and we will show that it carries a (possibly trivial) symplectic structure.

**Lemma 23.** *The set  $\text{Fix}_G(M)$  of fixed points in  $M$  under the action of the compact group  $G$  is a smooth symplectic submanifold of  $M$ .*

**Proof.** We notice first that the action of  $G$  on  $M$  induces a linear action of  $G$  on the vector space  $T_x M$  for each  $x \in \text{Fix}_G(M)$  denoted by  $g_* v$ ,  $g \in G$ ,  $v \in T_x M$ . Now it is simple to check that  $g_*$  defines a linear representation of  $G$  on  $T_x \text{Fix}_G(M)$  (in general it is easy to check that  $g_*$  defines a linear representation of  $G_x$  on  $T_x M$ ).

Now let us suppose that  $\text{Fix}_G(M)$  is not zero dimensional (in that case, the symplectic form will be trivial). On the other hand let us choose a  $G$ -invariant metric on  $M$  compatible with  $\omega$ . Such metric exists because the group  $Sp(2n, \mathbb{R})$  is contractible to the subgroup  $U(n)$ . Moreover, this allows to find and adapted

almost complex structure  $J$  for  $\omega$ , hence a metric  $\eta$  which is related to  $\omega$  by

$$\eta_x(u, v) = \omega_x(J_x u, v), \quad \forall u, v \in T_x M. \quad (107)$$

Then, averaging  $\eta$  and  $J$  over the group  $G$  we will find the demanded structures pointwise.

Let us take now a unitary eigenvector  $v$  of  $g_*$ . Consider now the linear function  $f_v: T_x M \rightarrow \mathbb{R}$  defined by  $f_v(u) = \eta_x(v, u)$ , for all  $u \in T_x M$ . Now the 1-form  $df_v = \hat{\eta}_x(v)$  defines a hamiltonian vector field  $X$  on  $T_x M$  via the symplectic structure  $\omega_x$ , i.e.

$$i_X \omega_x = df_v.$$

Because  $\omega_x$  and  $df_v$  are constant in  $T_x M$ , the same happens for  $X$  defining a constant tangent vector to  $T_x M$  that can be identified with a vector in  $T_x M$ . Let us denote such vector by  $v'$ . Then, computing  $\omega_x(v, v')$  we get

$$\omega_x(v', v) = i_X \omega_x(v) = df_v(v) = \eta_x(v, v) = 1.$$

On the other hand, it is clear that the covector  $df_v$  is an eigenvector of  $g_*$  with the same eigenvalue than  $v$  because both  $\eta_x, J$  are  $g_*$ -invariant. Hence, because  $\omega$  is also invariant with respect to  $g_*$ ,  $v'$  is an eigenvector with eigenvalue the same eigenvalue for the action of  $G$  on  $T_x M$ .

Thus we conclude that the pair  $v, v'$  just constructed span a symplectic subspace  $V$  of dimension 2 in  $T_x \text{Fix}_G(M)$ . Then we can take the orthogonal subspace  $V^\perp$  with respect to the metric  $\eta_x$  on  $T_x \text{Fix}_G(M)$  and repeat the argument.

Notice that because the compatibility property of  $\omega$  and  $\eta$ , Eq. (107), the restriction of  $\omega_x$  to  $V^\perp$  is symplectic too, thus the splitting  $T_x \text{Fix}_G(M) = V \oplus V^\perp$  is a symplectic splitting.  $\square$

Consider now  $L$  to be a Lagrangian submanifold of a symplectic manifold  $M$ . Let  $S$  be a symplectic submanifold of  $M$ . Weinstein's theorem on the local structure of Lagrangian embeddings asserts that there exists a tubular neighborhood of  $L$  on  $M$  symplectomorphic to a tubular neighborhood of  $L$  on  $T^*L$  as the zero section of the cotangent bundle. Then we can construct a Lagrangian foliation in the neighborhood of a given point  $x \in L$  by pulling back the (local) Lagrangian foliation of  $T^*L$  defined by a family of closed 1-forms  $\alpha_y$  parametrized by  $y$ , such that  $\alpha_0 = 0$ , in an open subset  $U \subset \mathbb{R}^n$ ,  $0 \in U$ ,  $n = \dim L$ .

Then, we will say that the Lagrangian submanifold  $L$  is transverse to the symplectic submanifold  $S$  at  $x \in L \cap S$  in the symplectic category if  $S$  is transverse to a local Lagrangian foliation in a neighborhood of  $x$  that contains  $L$ . We will say that  $L$  and  $S$  are symplectically transversal if they are transversal in the symplectic category at each  $x \in L \cap S$ . Such local foliation always exist by the previous remarks and the notion of symplectic transversality implies that the intersection  $L \cap S$  is a Lagrangian submanifold of  $S$ .

**Lemma 24.** *If the Lagrangian submanifold  $L$  and the symplectic submanifold are symplectically transversal, the intersection  $L \cap S$  is a Lagrangian submanifold of  $S$ .*

**Proof.** Because the submanifold  $S$  is transversal to a local foliation of  $M$  then the intersection with the leaves are submanifolds. In particular the intersection with  $L$  is a submanifold. This holds in a neighborhood of each point, than we have patches covering the intersection  $L \cap S$ . But it is clear from the definition of local foliation in the neighborhood of a point in  $L$  that this patches can be chosen to be contained in local coordinate neighborhoods of  $L$  hence they define on  $L$  the same differentiable structure.

It is obvious that  $L \cap S$  is an isotropic submanifold of  $M$ , hence it is isotropic of the symplectic submanifold  $S$ . Let now  $X$  be in  $T(S \cap L)^\perp$ . Then,  $\omega(X, Y) = 0$  for all  $Y \in T(S \cap L)$ . Because  $T(S \cap L) \subset TS$ , then  $TS^\perp \subset T(S \cap L)^\perp$ , but  $TS \oplus TS^\perp = TM$ .  $\square$

### 8.6. The reduction of the Grassmannian and the space of virtual self-adjoint extensions

We can apply the discussion in the previous section to the space of elliptic self-adjoint extensions. In fact, the space of elliptic self-adjoint extensions of the Dirac operator  $\mathcal{D}$ , the elliptic self-adjoint Grassmannian  $\mathcal{M}_{\text{ellip}}(\mathcal{D})$  is a Lagrangian submanifold of the infinite dimensional Grassmannian  $\text{Gr}(\mathcal{D})$ . Moreover the group  $G$  acts on  $\text{Gr}(\mathcal{D})$  because unitary representations of a compact group transform a closed subspace  $W$  into another one which still is in  $\mathbf{Gr}$ . In addition  $G$  acts on  $\mathbf{Gr}$  symplectically.

We can check this easily because in the dense subset of the Grassmannian made of subspaces  $W_T$  which are graphs of closed operators  $T$ , the group  $G$  acts as  $g \cdot W_T = W_{U(g)^\dagger T U(g)}$ . Hence the group  $G$  will act on tangent vectors  $\dot{A} \in T_{W_T} \mathbf{Gr}$ , as

$$g_* \dot{A} = U(g)^\dagger \dot{A} U(g).$$

The following computation shows that  $\omega_W$  is actually  $G$ -invariant (the subindex at  $\omega$  will be omitted):

$$\begin{aligned} \omega(g_* \dot{A}, g_* \dot{B}) &= \frac{i}{2} \text{Tr}((g_* \dot{A})^\dagger g_* \dot{B} - (g_* \dot{B})^\dagger g_* \dot{A}) \\ &= \frac{i}{2} \text{Tr}((U(g)^\dagger \dot{A} U(g))^\dagger U(g)^\dagger \dot{B} U(g) - (U(g)^\dagger \dot{B} U(g))^\dagger U(g)^\dagger \dot{A} U(g)) \\ &= \frac{i}{2} \text{Tr}(U(g)^\dagger \dot{A}^\dagger \dot{B} U(g) - U(g)^\dagger \dot{B}^\dagger \dot{A} U(g)) = \\ &= \frac{i}{2} \text{Tr}(\dot{A}^\dagger \dot{B} - \dot{B}^\dagger \dot{A}) = \omega(\dot{A}, \dot{B}). \end{aligned}$$

On the other hand, the fixed set of  $G$  in  $\text{Gr}(\mathcal{D})$  is formed precisely by the invariant subspaces in  $\text{Gr}(\mathcal{D})$ . That is,

$$\text{Fix}_G(\text{Gr}(\mathcal{D})) = \{ W \in \text{Gr}(\mathcal{D}) \mid g \cdot W = W, \forall g \in G \}.$$

Notice that if  $W = W_T$ , i.e.,  $W$  is the graph of the operator  $T$ , then  $g \cdot W = W$  iff  $U(g)T = TU(g)$ . That means that the set of fixed points under  $G$  is the closure in the Grassmannian of the set of  $G$ -invariant operators.

Moreover, because of Lemma 23,  $\text{Fix}_G(\text{Gr}(\mathcal{D}))$  is symplectic. On the other hand because of Thm. 11,  $\mathcal{M}_{\text{ellip}}(\mathcal{D})$  is a Lagrangian submanifold in  $\text{Gr}(\mathcal{D})$ . In addition both  $\mathcal{M}(\mathcal{D})$  and  $\mathcal{M}_{\text{ellip}}(\mathcal{D})$  are  $G$ -invariant. Obviously, if  $W$  is a self-adjoint subspace,  $g \cdot W$  is also self-adjoint because  $G$  acts unitarily in  $\mathcal{H}_D$ .

Finally, notice that  $\text{Fix}_G(\text{Gr}(\mathcal{D})) \cap \mathcal{M}_{\text{ellip}}(\mathcal{D}) = \text{Fix}_G(\mathcal{M}_{\text{ellip}}(\mathcal{D}))$ . Then, because of Lemma 24, we conclude that  $\text{Fix}_G(\mathcal{M}(\mathcal{D}))$  is a Lagrangian submanifold of  $\text{Fix}_G(\text{Gr}(\mathcal{D}))$  that will be denoted by  $\mathcal{M}_0$ . We have concluded the proof of the following theorem.

**Theorem 25.** *The space  $\text{Fix}_G(\text{Gr}(\mathcal{D}))$  of  $G$ -invariant subspaces of the Grassmannian  $\text{Gr}(\mathcal{D})$  is a symplectic submanifold. Moreover the space of  $G$ -invariant elliptic self-adjoint extensions of  $\mathcal{D}$  is a Lagrangian submanifold of  $\text{Fix}_G(\text{Gr}(\mathcal{D}))$ .*

As it was pointed before, the spaces  $\text{Fix}_G(\mathcal{M}_{\text{ellip}}(\mathcal{D}))$  and  $\text{Fix}_G(\mathcal{M}(\mathcal{D}))$  are closely related to the spaces of elliptic self-adjoint extensions and self-adjoint extensions of the quotient Dirac operator  $\mathcal{D}/G$  respectively, but they still consist of functions on  $\partial\Omega$  and not in  $\partial\Omega/G$ . In order to compare them we will have to relate  $\text{Gr}(\mathcal{H}_{D/G})$  with  $\text{Fix}_G(\mathcal{H}_D)$ . However that is easily done, noticing that on each  $G$ -invariant subspace  $W$  we can select the closed subspace made of  $G$ -invariant vectors, i.e., the eigenspace with eigenvalue 1 for the unitary representation of  $G$ . This space will be denoted by  $W^G$  and it coincides with the intersection  $W \cap \mathcal{H}_D^G$ .

**Proposition 26.** *For a compact group action of  $G$  on  $\Omega$  with smooth quotient space  $\Omega/G$  and a  $G$ -invariant Dirac operator  $\mathcal{D}$ , the spaces  $\text{Fix}_G(\mathcal{M}_{\text{ellip}}(\mathcal{D}))$  and  $\mathcal{M}_{\text{ellip}}(\mathcal{D}/G)$  are symplectically diffeomorphic.*

We conclude this discussion by remarking that even if the space  $\mathcal{H}_D^G$  of invariant vectors is always well defined for arbitrary  $G$ -actions on  $\Omega$ , it is not the same for  $\text{Gr}(\mathcal{D}/G)$  because if the space of leaves  $\Omega$  is singular, it is not obvious at all what is the meaning of  $\mathcal{D}/G$ .

Thus we define the space of ‘virtual elliptic self-adjoint extensions’ of the quotient Dirac operator  $\mathcal{D}/G$  as the family of closed subspaces in  $\text{Fix}_G(\mathcal{M}_{\text{ellip}}(\mathcal{D}))$ . We shall denote this space by  $\mathcal{M}(\mathcal{D}/G)$  and it is a Lagrangian submanifold of  $\text{Gr}(\mathcal{H}_D^G)$  whenever both are manifolds.

## 9. Spontaneous symmetry breaking and self-adjoint extensions

A basic ingredient in the construction of gauge invariant theories of interacting quantum fields was the discovery of the mechanism of spontaneous symmetry breaking that allowed to explain the mass spectrum of the theories [Go61], [Hi64].

### 9.1. The notion of spontaneous symmetry breaking

Spontaneous symmetry breaking has since then received a detailed analysis from the mathematical and physical viewpoints [Ki67], [We74]. L. Michel and L. Radicati in particular obtained the firsts theorems on the subject [Mi68], [Mi73] and a series of refinements and developments followed (see for instance [Ga97] and references therein).

Roughly speaking, spontaneous symmetry breaking happens when the equations describing a physical theory possess a given symmetry but the physical states of the theory have a smaller symmetry algebra. The way this situation is modeled in Quantum Field Theories is based on the fact that the symmetry of the Lagrangian has not to the same as the symmetry of the vacuum state of the theory. The specific mechanism that selects the physical vacuum stated among the orbits of the symmetry group of the theory on the Hilbert space of the quantum system is not clearly stated.

We will discuss a concrete mechanism of spontaneous symmetry breaking on our simplified model of first quantized quantum systems. The basic idea is extremely simple. As it was described in the previous section, for a given symmetry group  $G$ , invariant Dirac and Laplacian operators can be constructed. Thus the equations of the theory will be  $G$ -invariant. However, if the manifold of classical states, in our case  $\Omega$ , has a nontrivial boundary, the self-adjoint extensions of the operators could break this theory in the sense that the domain of the given self-adjoint extension will not be invariant under the group  $G$ .

As it was stated in Thm. 25 the elliptic self-adjoint extensions of the quotient Dirac operator  $\mathcal{D}/G$  are in one-to-one correspondence with the space  $\mathcal{M}_G(\mathcal{D})$ , the space of fixed points of the action of  $G$  on the space  $\mathcal{M}_{\text{ellip}}(\mathcal{D})$  of elliptic self-adjoint extensions of  $\mathcal{D}$ . Thus all subspaces in its complement are breaking the symmetry of the theory, in the sense that the functions in the corresponding domains not only do not have to be  $G$ -invariant, but that its transformed under  $G$  could lie out of the domain of the operator itself. Thus the operator  $\mathcal{D}_W$  defined by  $W$  not in  $\text{Fix}_G$  will of course commute with the action of  $G$ , but its spectrum will certainly not be  $G$ -invariant. We shall explore this idea in detail in what follows.

Let us consider for instance a simple example that will illustrate this idea. Consider the 1D free particle on the interval  $[-\pi, \pi]$  with Hamiltonian  $H = -d^2/dx^2$ . The parity group  $\mathbb{Z}_2$  acts on the Hilbert space  $L^2([-\pi, \pi])$  as  $P\Psi(x) = \Psi(-x)$  and clearly  $[P, H] = 0$  [Ag01]. However not all allowed self-adjoint extensions of the Hamiltonian operator are invariant with respect to  $P$ . Actually the space of self-adjoint extensions of  $H$  is parametrised by the unitary group  $U(2)$ . The induced



action on the boundary space Hilbert space  $\mathbb{C}_{-\pi} \oplus \mathbb{C}_{\pi}$ , where  $\mathbb{C}_{\pi}$  denotes the space of boundary values  $\psi_{\pm}^{\pi} = \Psi(\pi) \pm i\Psi'(\pi)$  and  $\mathbb{C}_{\pi}$ ,  $\psi_{\pm}^{-\pi} = \Psi(-\pi) \mp i\Psi'(-\pi)$  respectively. The element  $P$  acts on this space as the matrix

$$P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

hence, only those self-adjoint boundary conditions defined by unitary matrices of the form:

$$U(\alpha, \delta) = e^{i\delta} \begin{bmatrix} \cos \alpha & e^{i\pi/2} \sin \alpha \\ e^{i\pi/2} \sin \alpha & \cos \alpha \end{bmatrix},$$

will define domains invariant under  $P$ . Thus, for instance, quasi-periodic boundary conditions will break the symmetry  $P$ .

Another, less trivial, example in the same spirit is provided by a result by Falceto and Esteve on a generalization of the Virial Theorem [Es12]. Consider a free particle in one dimension restricted to move in  $[0, \infty)$  and subject to Robin boundary conditions, i.e.  $\Psi'(0) + \alpha\Psi(0) = 0$  with  $\alpha > 0$ . In this case the free Hamiltonian has a single eigenfunction  $\Psi_0(x) = \sqrt{2}\alpha e^{-\alpha x}$  with eigenvalue

$$E_0 = -\frac{\hbar^2 \alpha^2}{2m}.$$

If we use the Virial Theorem:

$$2\langle \Psi_0 | T | \Psi_0 \rangle = \langle \Psi_0 | xV'(x) | \Psi_0 \rangle,$$

to compute the expectation value of the kinetic energy in this state we obtain that it vanishes, which is in contradiction with the real result:

$$\langle \Psi_0 | T | \Psi_0 \rangle = E_0.$$

The reason for this apparent contradiction is the fact that the domain of the Hamiltonian is not preserved by the generator of the group of scale transformations

$$E = -\frac{i}{\hbar}xp - \frac{1}{2},$$

and the virial theorem has to be modified.

The group theoretical analysis of this example is as follows. The group  $G$  of scale transformations acts on the space of  $L^2(\mathbb{R}^+)$  functions as:

$$(\delta_s \Psi)(x) = e^{s/2} \Psi(e^s x), \quad s \in \mathbb{R}, x \in \mathbb{R}^+.$$

Notice that this action defines a unitary representation of the group as:  $\|\delta_s \Psi\| = \|\Psi\|$  for all  $s \in \mathbb{R}$ ,  $\Psi \in L^2(\mathbb{R}^+)$ . The free particle Hamiltonian operator  $H_0$  transforms under the action of  $\delta_s$  as:

$$\delta_s^{-1} H_0 \delta_s = e^{2s} H_0,$$

thus the virial theorem is obtained by observing that

$$\begin{aligned}\langle \Psi_n | [H, E] | \Psi_n \rangle &= \langle \Psi_n | HE | \Psi_n \rangle - \langle \Psi_n | EH | \Psi_n \rangle \\ &= \langle H\Psi_n | E | \Psi_n \rangle - \langle \Psi_n | EH | \Psi_n \rangle = 0,\end{aligned}$$

where  $H$  is a self-adjoint operator with domain  $D(H)$ ,  $|\Psi_n\rangle$  is an eigenvector, and  $E|\Psi_n\rangle$  must lie in the domain of  $H$ . However if  $E|\Psi_n\rangle \notin D(H)$  then the theorem fails. In the situation above, it is easy to realise that the vector  $E(\Psi_0)$  will not be in the domain  $D_\alpha \subset L^2(\mathbb{R}^+)$  defined by Robin's boundary conditions, because  $(\delta_s \Psi)(0) = e^{s/2} \Psi(0)$ , whereas  $(\delta_s \Psi')(0) = \Psi'(0)$ , hence if  $\Psi \in D_\alpha$ ,  $\alpha \neq 0$ , then  $\delta_s \Psi \in D_{e^{s/2}\alpha} \neq D_\alpha$ .

### 9.2. The bifurcation diagram of the space of self-adjoint extensions

We will analyze now in more detail the structure of the Lagrangian Grassmannian  $\mathcal{L}_{\not{D}}$  of the  $G$ -invariant Dirac operator  $\not{D}$ .

Let us recall that the action of the group  $G$  induces an action on subspaces of the boundary data Hilbert space  $\not{D}$ , hence it induces an action on the space of self-adjoint extensions  $\mathcal{M}_{\not{D}}$  of  $\not{D}$ . Moreover it also induces an action on the elliptic Grassmannian  $\text{Gr}(\not{D})$ . Notice that because the representation  $V$  of the group is unitary and continuous, then the transformed of a given subspace  $W^g = V(g)^\dagger W V(g)$  will have Fredholm and Hilbert-Schmidt projections on the corresponding polarization. Hence the action of  $G$  will map the elliptic self-adjoint Grassmannian  $\mathcal{L}_{\not{D}}$  onto itself.

The action of  $G$  on  $\mathcal{L}_{\not{D}}$  will induce a stratified structure on this manifold. If we denote by  $G_W$  the isotropy group of the vector subspace  $W \in \mathcal{L}_{\not{D}}$ , all the subspaces whose isotropy groups will lie in the conjugacy class of  $G_W$  will constitute a submanifold, the stratum  $\mathcal{O}_W$  of  $\mathcal{L}_{\not{D}}$ .

The fixed point set, i.e., the strictly invariant subspaces, that correspond to self-adjoint extensions of the reduced Dirac operator, define the minimal stratum  $\mathcal{O}_{\min} = \text{Fix}_G(\mathcal{L}_{\not{D}})$ , and the set of completely non-invariant subspaces, i.e., those subspaces  $W$  such that  $W^g \cap W = \mathbf{0}$ , constitute the maximal strata denoted by  $\mathcal{O}_{\max}$ . It is noticeable that  $\mathcal{O}_{\max}$  is an open dense submanifold of  $\mathcal{L}_{\not{D}}$ .

The manifold  $\mathcal{L}_{\not{D}}$  is decomposed then as a union

$$\text{Gr}(\mathcal{H}_D) = \cup_\alpha \mathcal{O}_\alpha,$$

of the different strata  $\mathcal{O}_\alpha$  labeled by an index  $\alpha$  that runs over the conjugacy classes of subgroups of  $G$ . The decomposition above is such that the boundary of any stratum is a union of strata,

$$\partial \mathcal{O}_\alpha = \cup_{\alpha'} \mathcal{O}_{\alpha'},$$

and under generic conditions, the strata  $\mathcal{O}_\alpha$  are submanifolds with boundary given by the expression above.

A partial ordering can be defined on the space of strata as follows  $\mathcal{O}_\alpha \prec \mathcal{O}_\beta$  if  $\mathcal{O}_\alpha \subset \partial\mathcal{O}_\beta$ . This partial relation induces a natural partial ordering in the space of conjugacy classes of subgroups of  $G$  which non-void strata. Denoting by  $G_\alpha$  a representative of the conjugacy class of subgroups of the strata  $\mathcal{O}_\alpha$ , we will define  $G_\alpha \prec G_\beta$  iff  $\mathcal{O}_\alpha \prec \mathcal{O}_\beta$  or, in other words, that is  $\alpha \prec \beta$  iff  $\mathcal{O}_\beta \prec \mathcal{O}_\alpha$ . The lattice of subgroups  $\{G_\alpha\}$  with the partial order  $\prec$  will be called the bifurcation diagram of the  $G$ -invariant operator  $\mathcal{D}$ .

The bifurcation diagram of  $\mathcal{D}$  represents the possible schemes of breaking the symmetry  $G$ . The subgroups  $G_\alpha \prec G_\beta$  can actually be chosen to be closed subgroups of each other, hence, for finite-dimensional Lie groups, the bifurcation diagram will necessarily have a finite number of levels (the maximum number of subgroups needed to go from the trivial group to  $G$ ).

The intersection of the space  $\mathcal{M}(\mathcal{D})$  of self-adjoint extensions of  $\mathcal{D}$  with the corresponding strata  $\mathcal{O}_\alpha$  will describe the self-adjoint extensions of  $\mathcal{D}$  with symmetry group  $G_\alpha$  determined by the boundary conditions. We will say that the symmetry is broken from  $G_\alpha$  to  $G_\beta$  if there is a change from the boundary conditions on  $\mathcal{O}_\beta \subset \partial\mathcal{O}_\alpha$  to the interior of  $\mathcal{O}_\alpha$ .

The problem of understanding such symmetry breaking is to describe how the properties of the operators  $\mathcal{D}_W$  change when  $W$  changes from  $\mathcal{O}_\beta$  to  $\mathcal{O}_\alpha$ , e.g., how their spectral invariants change.

We will only describe here the breaking from the trivial symmetry to  $G$ , i.e., from the minimal strata to the maximal one. Notice that this can always be done because  $\mathcal{O}_{\min} \subset \partial\mathcal{O}_{\max}$  and  $\mathcal{O}_{\max}$  is a dense open submanifold.

We denote by  $W$  a small generic perturbation of a  $G$ -invariant subspace  $W_0$ , i.e.,  $W \in \mathcal{O}_{\max}$ , and  $W^g \cap W = \mathbf{0}$  for all  $g \in G$ . Let  $\xi$  a section in the domain of  $\mathcal{D}_W$ , i.e.,  $\xi|_{\partial\Omega} \in W$ . Then defining a new variable  $\theta = \xi - \xi_0$  where  $\xi_0$  is a lowest positive eigenvalue solution of the eigenvalue equation  $\mathcal{D}_W \xi = m\xi$ , we obtain that the spectral equation for  $\mathcal{D}_W$  becomes the inhomogeneous equation for  $\theta$ :

$$\mathcal{D}\theta = E\theta + (E - m_0)\xi_0$$

and  $\theta|_{\partial\Omega} = 0$ , that is Dirichlet's boundary conditions which are always symmetric boundary condition. Thus the bifurcation  $G$  to  $e$  modifies the operator  $\mathcal{D}$  adding a nontrivial inhomogeneous term.

## 10. Conclusions and further developments

Unfortunately there is no room in these notes to discuss many other examples and problems from quantum systems involving boundary conditions and/or (non-)self-adjoint extension that deserve a detailed analysis and for which some of the results and ideas presented are relevant. We will just quote some of them.

The physical role, generation and control of edges states is paramount among them. We have briefly discussed how edge states are formed when approaching the Cayley surface, however a more detailed analysis is needed.

Close to this is the relation between topology change and dynamics of boundary conditions. Notice that states corresponding to boundary conditions close to the Cayley manifold can exhibit (when considered in a Quantum Field Theory) quantum corrections corresponding to changes in the topology of the underlying space. Again, these aspects should be investigated further.

The theory of self-adjoint extensions of Laplace or Dirac operators on manifolds with singularities, arising either from group actions or by suitable boundary conditions, like orbifolds, quantum systems with meromorphic or distributional, like  $\delta'$ , potentials, etc.

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80 *M. Asorey, A. Iborr, G. Marmo*

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